



Full wwPDB EM Validation Report ⓘ

Apr 6, 2026 – 01:16 AM UTC

PDB ID : 9M7Q / pdb_00009m7q
EMDB ID : EMD-63690
Title : Structure of flagellar hook at 3.18 angstroms resolution, conformation 1.
Authors : Chen, L.X.; Jiang, W.X.; Cheng, X.Q.; Dong, X.; Xing, Q.
Deposited on : 2025-03-11
Resolution : 3.18 Å (reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

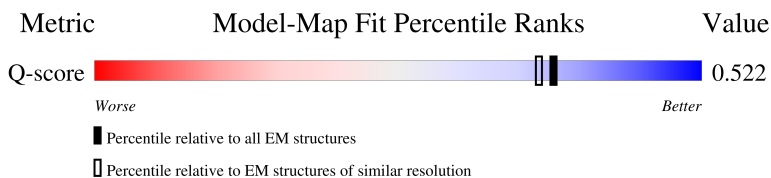
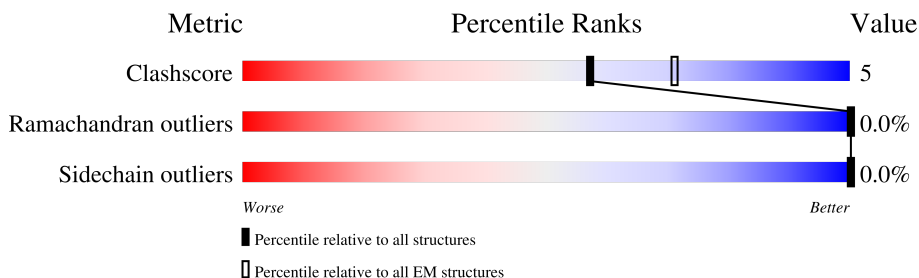
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY


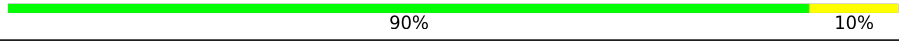
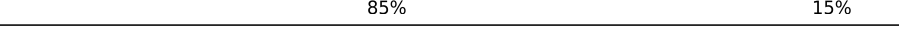

The reported resolution of this entry is 3.18 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




























Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14470 (2.68 - 3.68)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	DA	402	
1	DB	402	
1	DC	402	
1	DD	402	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	DE	402	 85%15%
1	DF	402	 86%14%
1	DG	402	 89%11%
1	DH	402	 90%10%
1	DI	402	 88%12%
1	DJ	402	 87%13%
1	DK	402	 86%14%
1	EA	402	 90%10%
1	EB	402	 89%11%
1	EC	402	 87%13%
1	ED	402	 92%8%
1	EE	402	 89%11%
1	EF	402	 90%10%
1	EG	402	 91%9%
1	EH	402	 86%14%
1	EI	402	 87%13%
1	EJ	402	 84%16%
1	EK	402	 87%13%
1	FA	402	 89%11%
1	FB	402	 91%9%
1	FC	402	 91%9%
1	FD	402	 92%8%
1	FE	402	 92%8%
1	FF	402	 87%13%
1	FG	402	 87%12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	FH	402	 88% 12%
1	FI	402	 86% 14%
1	FJ	402	 85% 15%
1	FK	402	 88% 12%
1	GA	402	 89% 11%
1	GB	402	 84% 16%
1	GC	402	 87% 13%
1	GD	402	 86% 14%
1	GE	402	 90% 10%
1	GF	402	 85% 15%
1	GG	402	 87% 13%
1	GH	402	 82% 18%
1	GI	402	 92% 8%
1	GJ	402	 86% 14%
1	GK	402	 93% 7%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 130196 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Flagellar hook protein FlgE.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	DA	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	DB	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	DC	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	DD	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	DE	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	DF	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	DG	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	DH	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	DI	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	DJ	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	DK	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	EA	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	EB	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	EC	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	ED	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	EE	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	EF	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	EG	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	EH	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	EI	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	EJ	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	EK	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	FA	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	FB	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	FC	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	FD	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	FE	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	FF	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	FG	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	FH	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	FI	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	FJ	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	FK	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	GA	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	GB	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	GC	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	GD	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	GE	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		

Continued on next page...

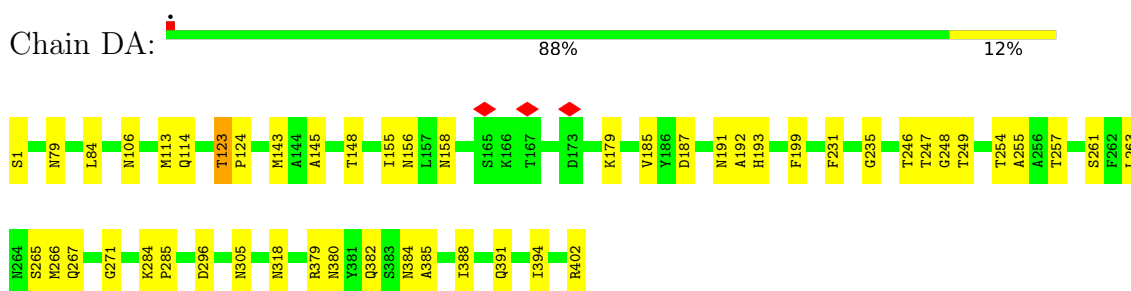
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	GF	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	GG	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	GH	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	GI	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	GJ	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		
1	GK	402	Total	C	N	O	S	0	0
			2959	1820	511	620	8		

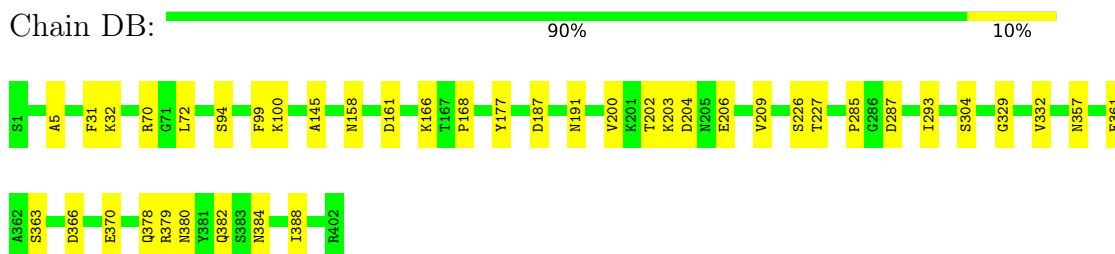
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

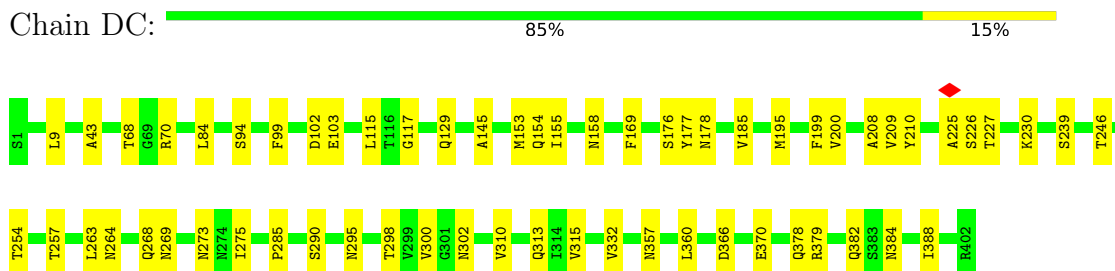
- Molecule 1: Flagellar hook protein FlgE



- Molecule 1: Flagellar hook protein FlgE



- Molecule 1: Flagellar hook protein FlgE



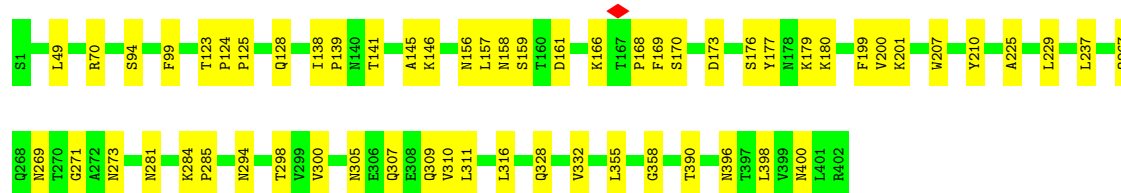
- Molecule 1: Flagellar hook protein FlgE





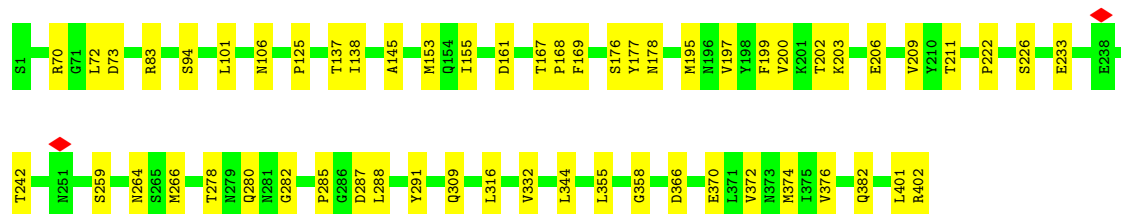
- Molecule 1: Flagellar hook protein FlgE

Chain DE: 85% 15%



- Molecule 1: Flagellar hook protein FlgE

Chain DF: 86% 14%



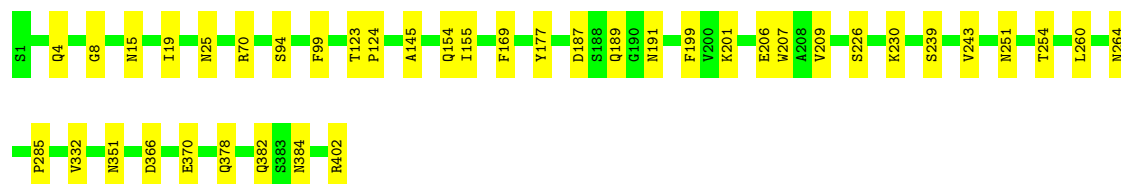
- Molecule 1: Flagellar hook protein FlgE

Chain DG: 89% 11%




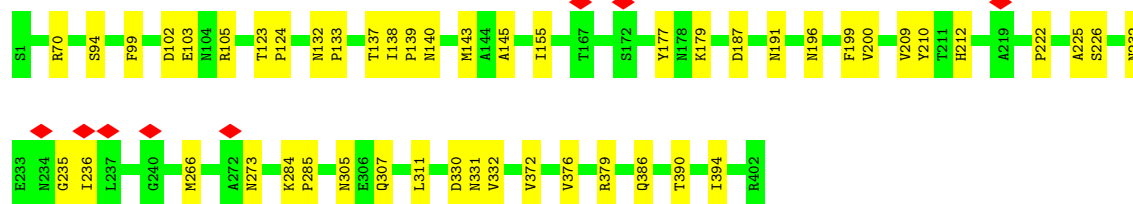
- Molecule 1: Flagellar hook protein FlgE

Chain DH: 90% 10%




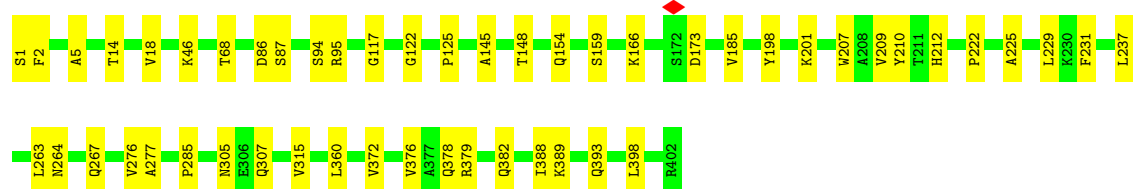
- Molecule 1: Flagellar hook protein FlgE

Chain DI:  88% 12%



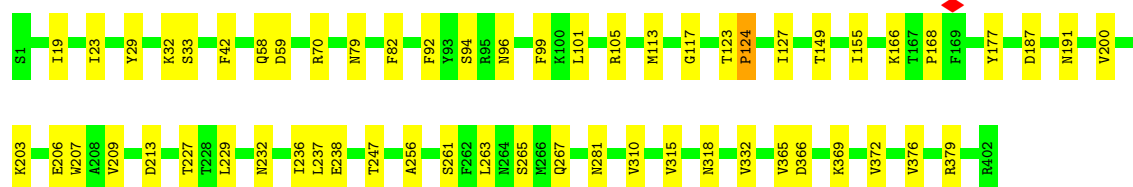
- Molecule 1: Flagellar hook protein FlgE

Chain DJ:  87% 13%



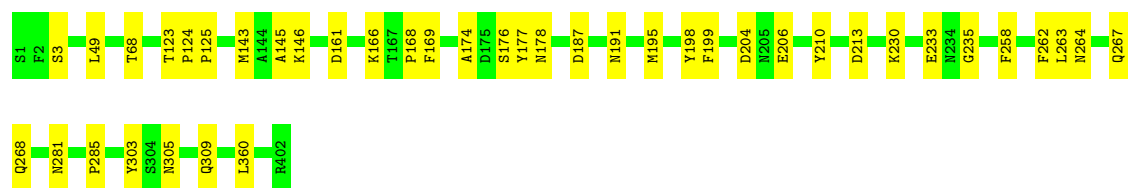
- Molecule 1: Flagellar hook protein FlgE

Chain DK:  86% 14%



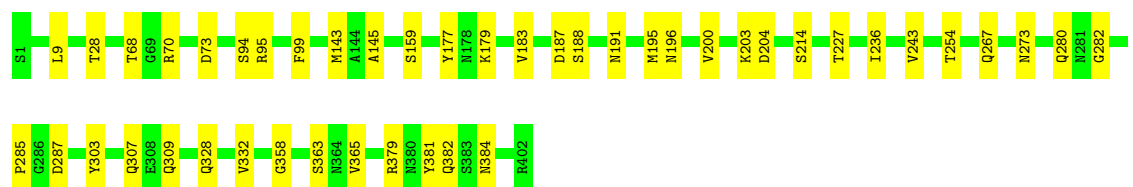
- Molecule 1: Flagellar hook protein FlgE

Chain EA:  90% 10%

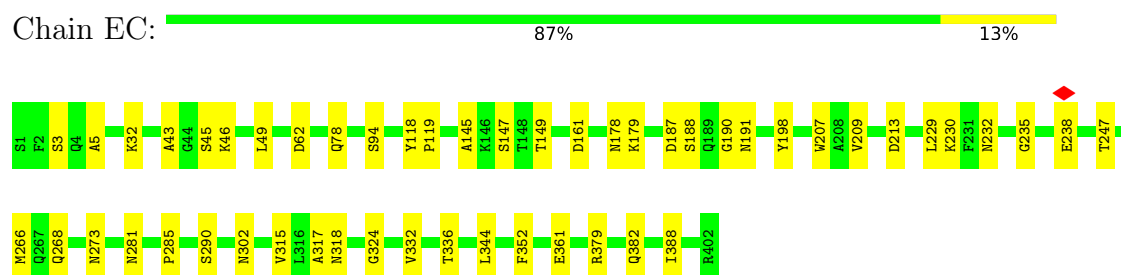


- Molecule 1: Flagellar hook protein FlgE

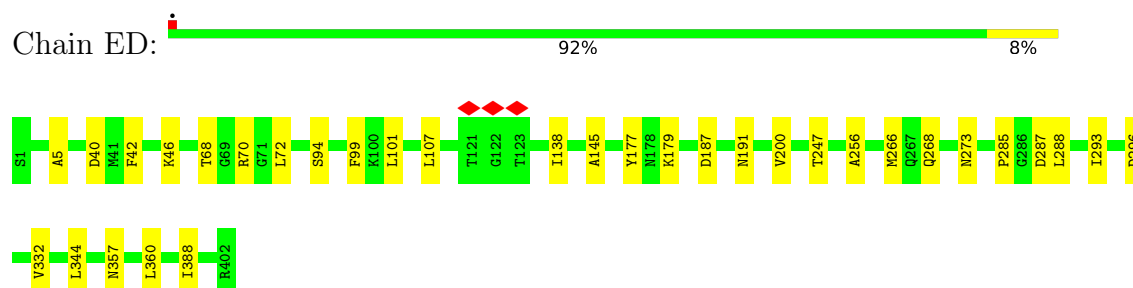
Chain EB:  89% 11%



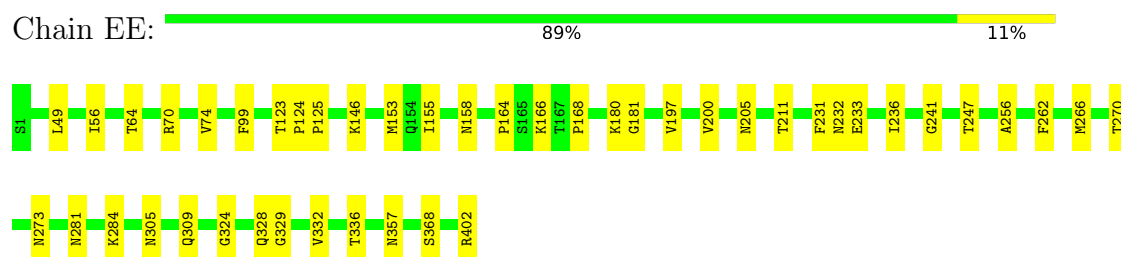
- Molecule 1: Flagellar hook protein FlgE



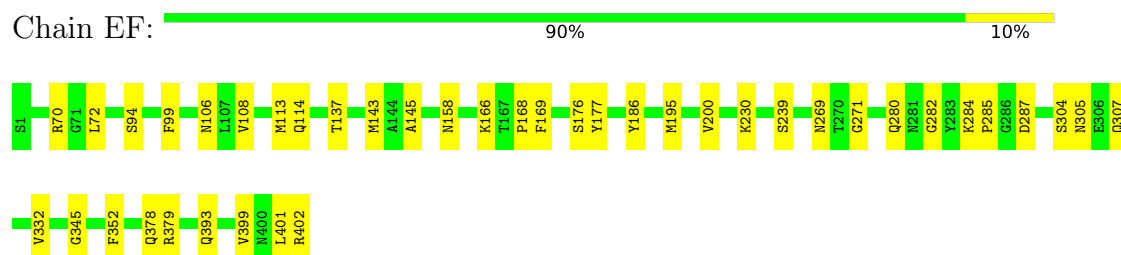
- Molecule 1: Flagellar hook protein FlgE



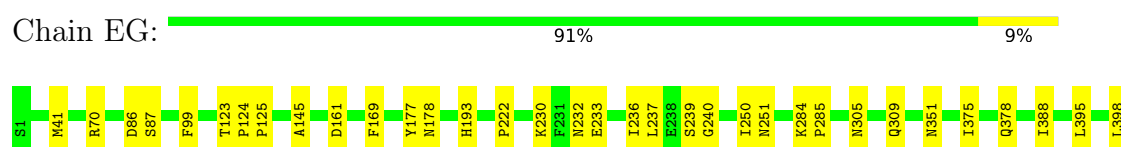
- Molecule 1: Flagellar hook protein FlgE



- Molecule 1: Flagellar hook protein FlgE



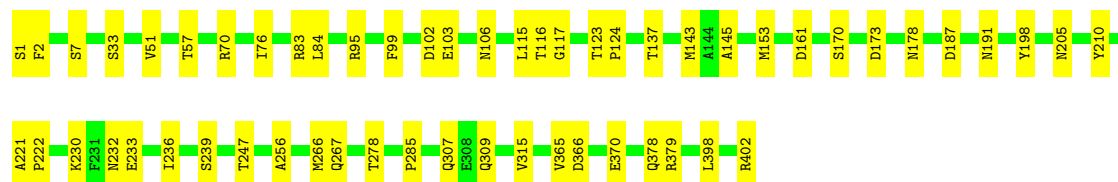
- Molecule 1: Flagellar hook protein FlgE





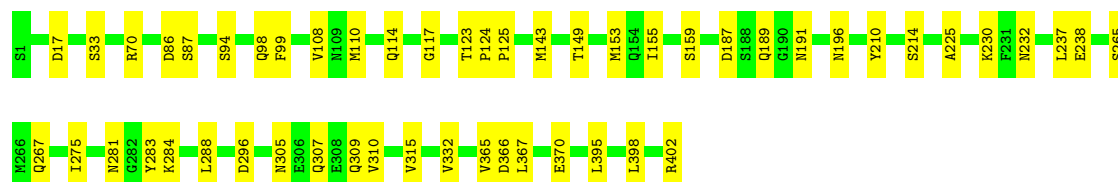
- Molecule 1: Flagellar hook protein FlgE

Chain EH: 86% 14%



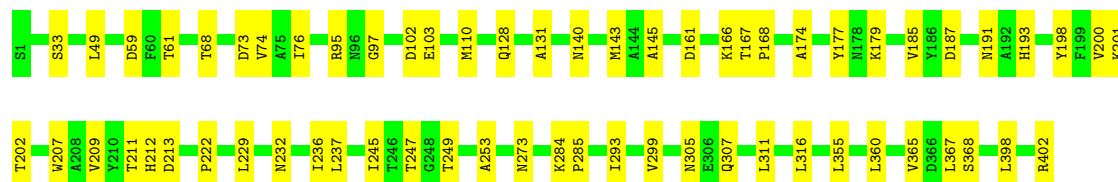
- Molecule 1: Flagellar hook protein FlgE

Chain EI: 87% 13%



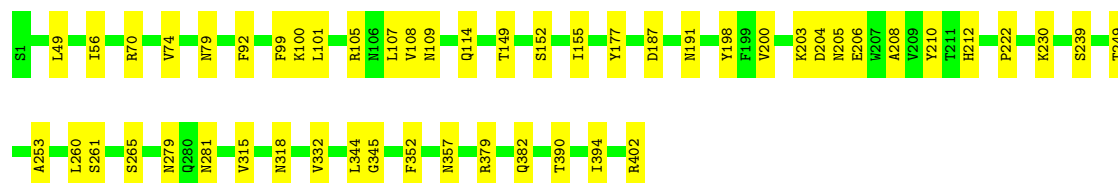
- Molecule 1: Flagellar hook protein FlgE

Chain EJ: 84% 16%



- Molecule 1: Flagellar hook protein FlgE

Chain EK: 87% 13%



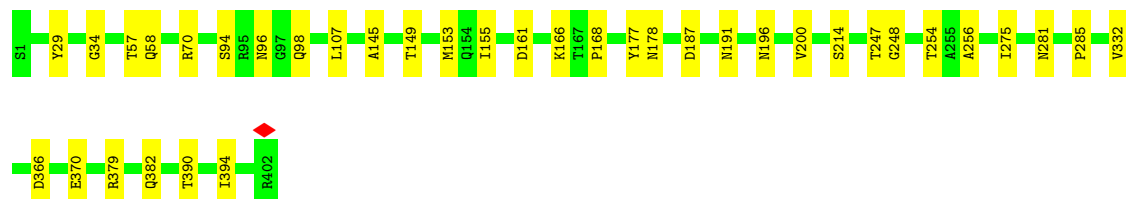
- Molecule 1: Flagellar hook protein FlgE

Chain FA: 89% 11%



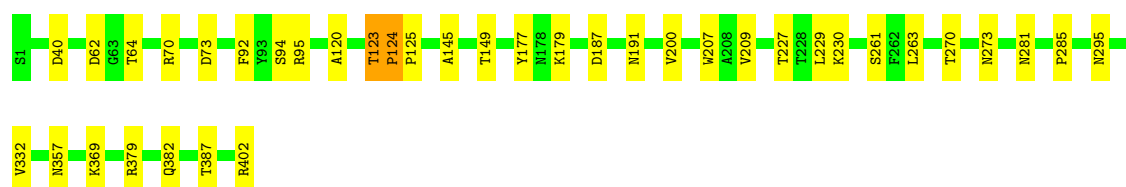
- Molecule 1: Flagellar hook protein FlgE

Chain FB: 91% 9%



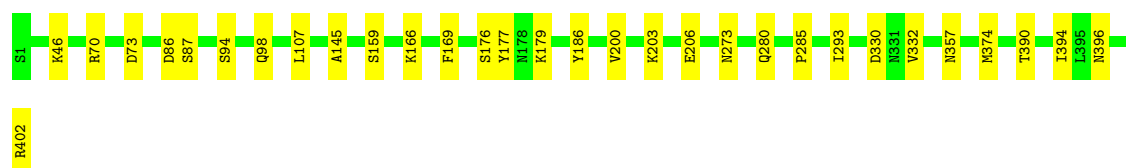
- Molecule 1: Flagellar hook protein FlgE

Chain FC: 91% 9%



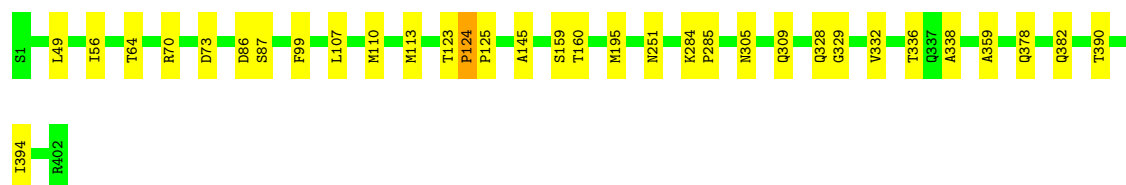
- Molecule 1: Flagellar hook protein FlgE

Chain FD: 92% 8%




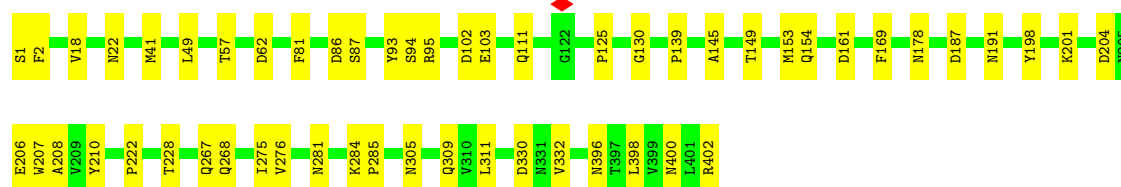
- Molecule 1: Flagellar hook protein FlgE

Chain FE: 92% 8%




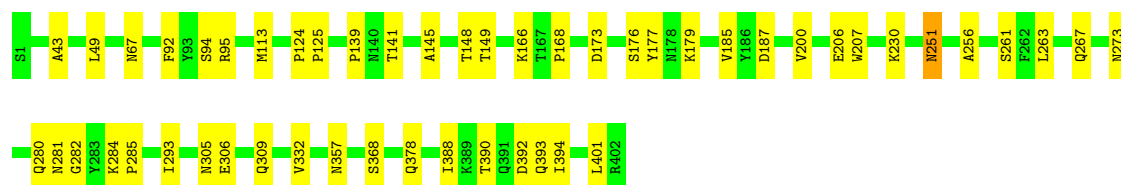
- Molecule 1: Flagellar hook protein FlgE

Chain FF:  87% 13%



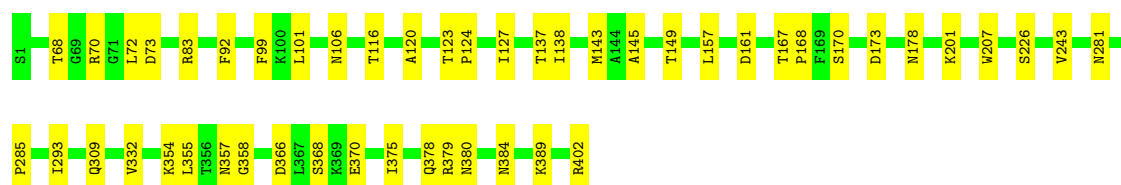
- Molecule 1: Flagellar hook protein FlgE

Chain FG:  87% 12%




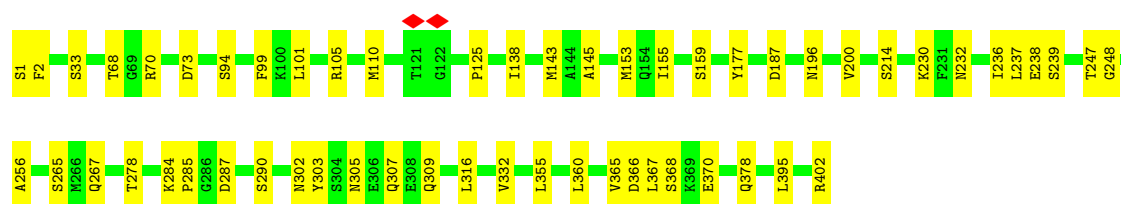
- Molecule 1: Flagellar hook protein FlgE

Chain FH:  88% 12%




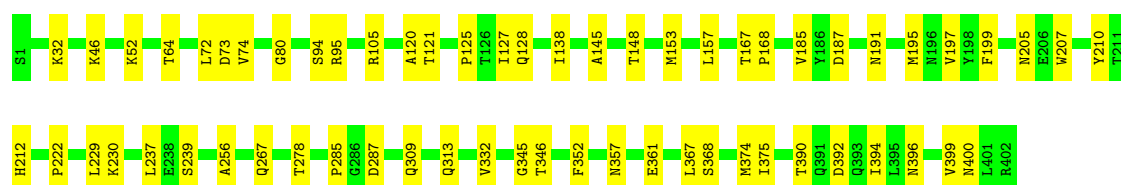
- Molecule 1: Flagellar hook protein FlgE

Chain FI:  86% 14%

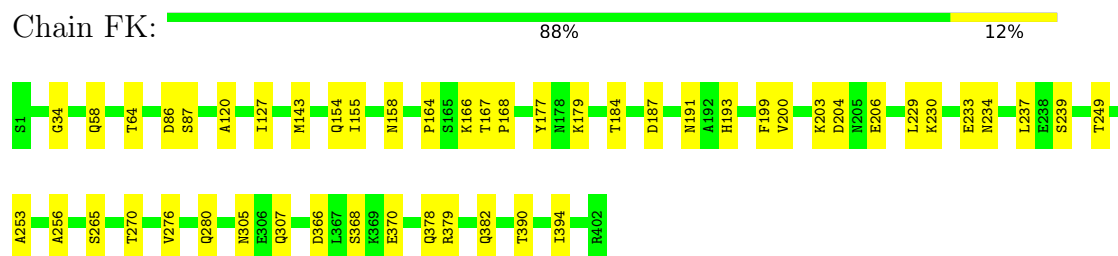


- Molecule 1: Flagellar hook protein FlgE

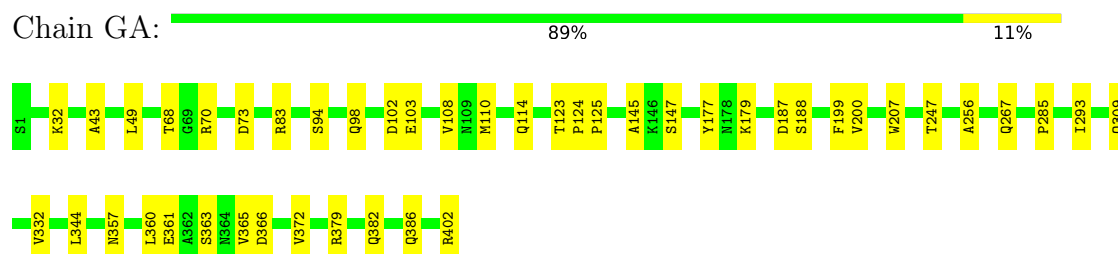
Chain FJ:  85% 15%



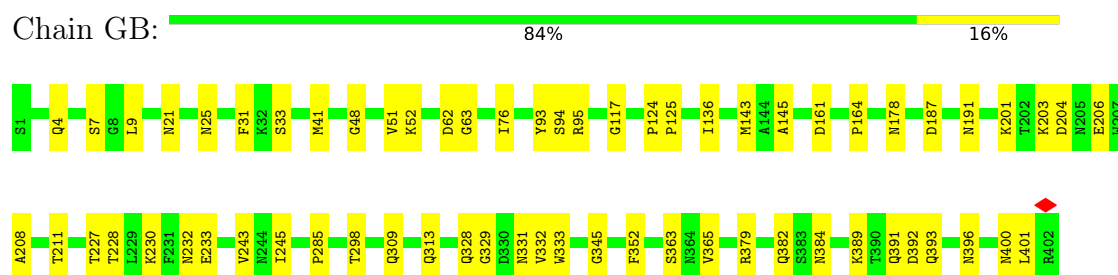
- Molecule 1: Flagellar hook protein FlgE



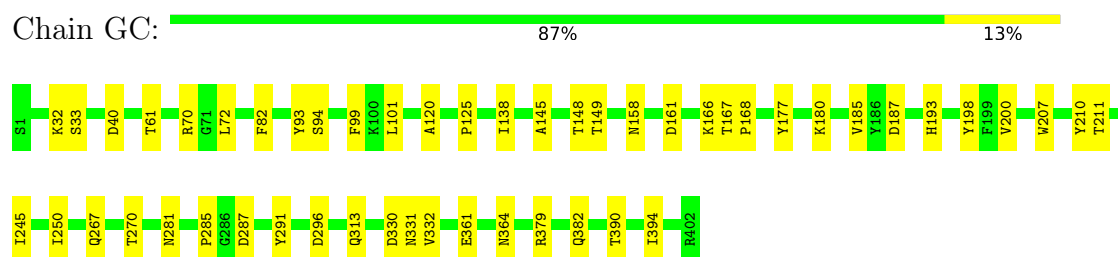
- Molecule 1: Flagellar hook protein FlgE



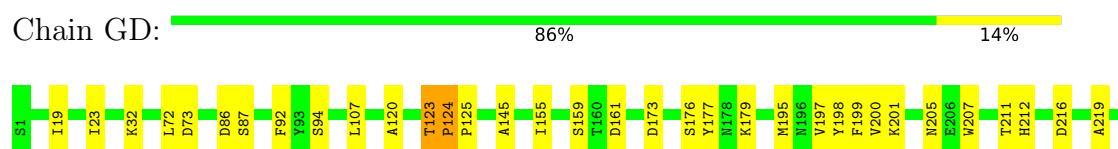
- Molecule 1: Flagellar hook protein FlgE



- Molecule 1: Flagellar hook protein FlgE



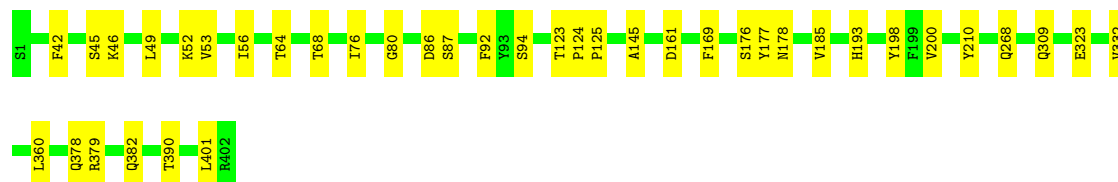
- Molecule 1: Flagellar hook protein FlgE





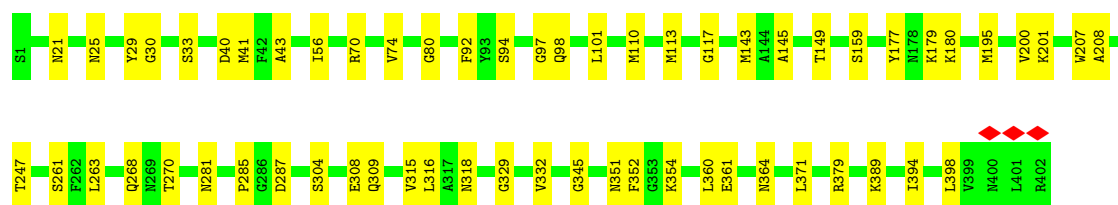
- Molecule 1: Flagellar hook protein FlgE

Chain GE: 90% 10%



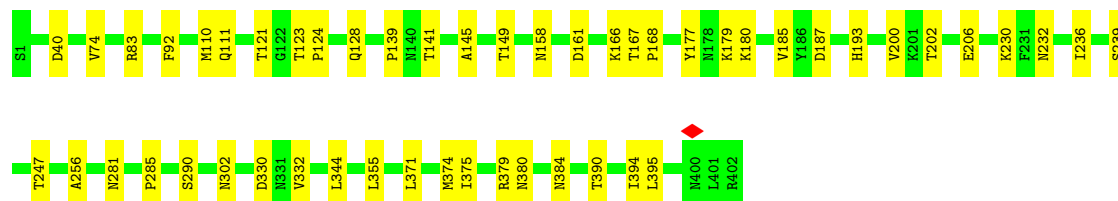
- Molecule 1: Flagellar hook protein FlgE

Chain GF: 85% 15%



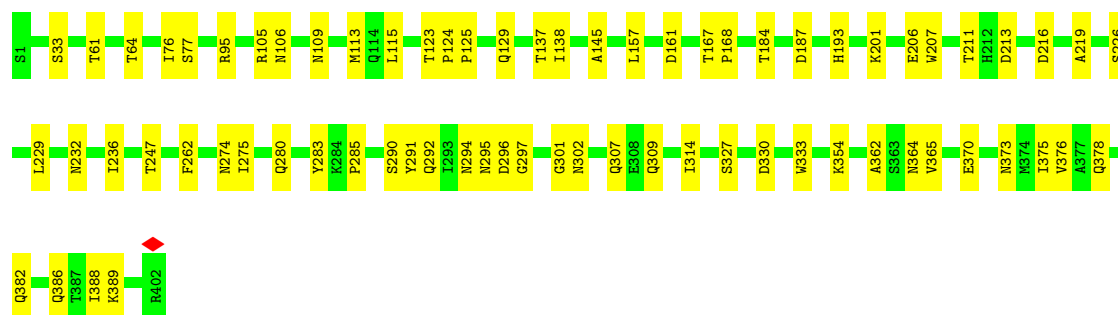
- Molecule 1: Flagellar hook protein FlgE

Chain GG: 87% 13%



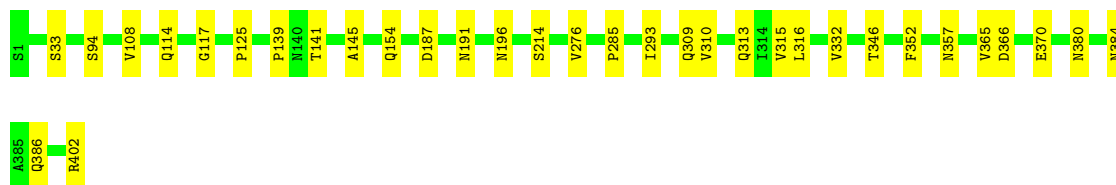
- Molecule 1: Flagellar hook protein FlgE

Chain GH: 82% 18%




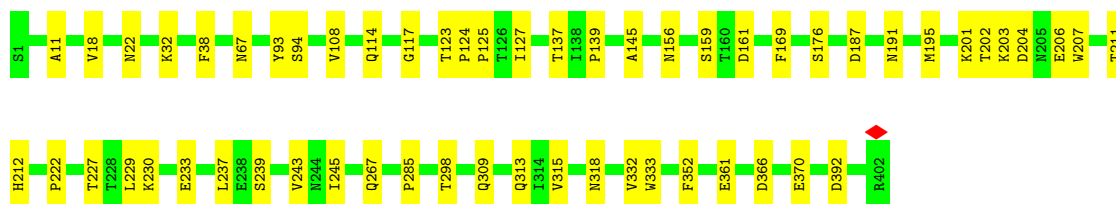
- Molecule 1: Flagellar hook protein FlgE

Chain GI:  92% 8%



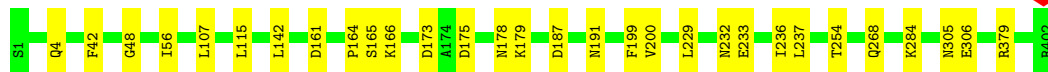
- Molecule 1: Flagellar hook protein FlgE

Chain GJ:  86% 14%



- Molecule 1: Flagellar hook protein FlgE

Chain GK:  93% 7%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	435796	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.123	Depositor
Minimum map value	-0.634	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.075	Depositor
Map size (\AA)	510.0, 510.0, 510.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.85, 0.85, 0.85	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	DA	0.11	0/3003	0.31	0/4090
1	DB	0.10	0/3003	0.27	0/4090
1	DC	0.11	0/3003	0.28	0/4090
1	DD	0.12	0/3003	0.30	0/4090
1	DE	0.11	0/3003	0.29	0/4090
1	DF	0.11	0/3003	0.28	0/4090
1	DG	0.13	0/3003	0.32	1/4090 (0.0%)
1	DH	0.11	0/3003	0.28	0/4090
1	DI	0.12	0/3003	0.28	0/4090
1	DJ	0.11	0/3003	0.31	0/4090
1	DK	0.13	0/3003	0.31	2/4090 (0.0%)
1	EA	0.09	0/3003	0.28	0/4090
1	EB	0.09	0/3003	0.25	0/4090
1	EC	0.09	0/3003	0.26	0/4090
1	ED	0.09	0/3003	0.25	0/4090
1	EE	0.09	0/3003	0.25	0/4090
1	EF	0.08	0/3003	0.26	0/4090
1	EG	0.09	0/3003	0.25	0/4090
1	EH	0.09	0/3003	0.26	0/4090
1	EI	0.10	0/3003	0.26	0/4090
1	EJ	0.09	0/3003	0.25	0/4090
1	EK	0.09	0/3003	0.26	0/4090
1	FA	0.09	0/3003	0.27	0/4090
1	FB	0.09	0/3003	0.25	0/4090
1	FC	0.09	0/3003	0.24	0/4090
1	FD	0.09	0/3003	0.25	0/4090
1	FE	0.09	0/3003	0.26	0/4090
1	FF	0.09	0/3003	0.26	0/4090
1	FG	0.09	0/3003	0.26	0/4090
1	FH	0.08	0/3003	0.22	0/4090
1	FI	0.09	0/3003	0.25	0/4090
1	FJ	0.09	0/3003	0.24	0/4090
1	FK	0.09	0/3003	0.26	0/4090
1	GA	0.10	0/3003	0.27	0/4090

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	GB	0.08	0/3003	0.24	0/4090
1	GC	0.09	0/3003	0.25	0/4090
1	GD	0.10	0/3003	0.28	0/4090
1	GE	0.08	0/3003	0.25	0/4090
1	GF	0.09	0/3003	0.26	0/4090
1	GG	0.09	0/3003	0.24	0/4090
1	GH	0.10	0/3003	0.28	0/4090
1	GI	0.08	0/3003	0.24	0/4090
1	GJ	0.09	0/3003	0.26	0/4090
1	GK	0.09	0/3003	0.26	0/4090
All	All	0.10	0/132132	0.27	3/179960 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	DA	0	1
1	DD	0	1
1	FC	0	1
1	FE	0	1
1	GD	0	1
All	All	0	5

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DK	124	PRO	CA-N-CD	-5.59	103.67	111.50
1	DK	124	PRO	N-CD-CG	-5.33	97.41	103.80
1	DG	222	PRO	CA-N-CD	-5.23	104.67	112.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	DA	123	THR	Peptide
1	DD	124	PRO	Peptide
1	FC	123	THR	Peptide
1	FE	124	PRO	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	GD	123	THR	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	DA	2959	0	2855	30	0
1	DB	2959	0	2855	22	0
1	DC	2959	0	2855	41	0
1	DD	2959	0	2855	23	0
1	DE	2959	0	2855	38	0
1	DF	2959	0	2855	37	0
1	DG	2959	0	2855	31	0
1	DH	2959	0	2855	30	0
1	DI	2959	0	2855	27	0
1	DJ	2959	0	2855	28	0
1	DK	2959	0	2855	33	0
1	EA	2959	0	2855	27	0
1	EB	2959	0	2855	29	0
1	EC	2959	0	2855	31	0
1	ED	2959	0	2855	20	0
1	EE	2959	0	2855	29	0
1	EF	2959	0	2855	27	0
1	EG	2959	0	2855	26	0
1	EH	2959	0	2855	33	0
1	EI	2959	0	2855	33	0
1	EJ	2959	0	2855	38	0
1	EK	2959	0	2855	30	0
1	FA	2959	0	2855	30	0
1	FB	2959	0	2855	23	0
1	FC	2959	0	2855	26	0
1	FD	2959	0	2855	22	0
1	FE	2959	0	2855	23	0
1	FF	2959	0	2855	31	0
1	FG	2959	0	2855	35	0
1	FH	2959	0	2855	32	0
1	FI	2959	0	2855	35	0
1	FJ	2959	0	2855	42	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	FK	2959	0	2855	30	0
1	GA	2959	0	2855	26	0
1	GB	2959	0	2855	39	0
1	GC	2959	0	2855	34	0
1	GD	2959	0	2855	34	0
1	GE	2959	0	2855	26	0
1	GF	2959	0	2855	38	0
1	GG	2959	0	2855	31	0
1	GH	2959	0	2855	43	0
1	GI	2959	0	2855	19	0
1	GJ	2959	0	2855	33	0
1	GK	2959	0	2855	19	0
All	All	130196	0	125620	1227	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (1227) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GD:19:ILE:HG23	1:GD:370:GLU:HB3	1.62	0.80
1:DF:125:PRO:HG2	1:DF:309:GLN:HB2	1.68	0.76
1:DK:32:LYS:HB2	1:DK:58:GLN:HE21	1.51	0.74
1:DJ:86:ASP:OD1	1:DJ:87:SER:N	2.21	0.74
1:EI:86:ASP:OD1	1:EI:87:SER:N	2.21	0.74
1:DI:284:LYS:O	1:DI:305:ASN:ND2	2.18	0.73
1:GA:102:ASP:OD1	1:GA:103:GLU:N	2.22	0.72
1:EG:86:ASP:OD2	1:EG:87:SER:N	2.23	0.72
1:GG:166:LYS:HG3	1:GG:168:PRO:HD2	1.72	0.72
1:EA:145:ALA:HB2	1:EA:285:PRO:HD3	1.71	0.72
1:GH:125:PRO:HG2	1:GH:309:GLN:HB2	1.72	0.71
1:DF:203:LYS:HE2	1:DF:206:GLU:HG3	1.72	0.71
1:DK:79:ASN:OD1	1:DK:318:ASN:ND2	2.23	0.71
1:DE:166:LYS:HG2	1:DE:168:PRO:HD2	1.74	0.70
1:EB:70:ARG:NH2	1:EB:99:PHE:O	2.24	0.70
1:EE:164:PRO:HG2	1:EE:200:VAL:HG23	1.74	0.70
1:DB:70:ARG:NH2	1:DB:99:PHE:O	2.25	0.69
1:EI:125:PRO:HG2	1:EI:309:GLN:HB2	1.74	0.69
1:DC:177:TYR:HA	1:DC:200:VAL:HG12	1.75	0.69
1:DF:153:MET:HE2	1:DF:155:ILE:HD11	1.74	0.69
1:DF:161:ASP:OD2	1:DF:178:ASN:ND2	2.25	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EC:290:SER:OG	1:EC:302:ASN:ND2	2.26	0.69
1:EH:102:ASP:OD1	1:EH:103:GLU:N	2.26	0.69
1:FK:166:LYS:HG3	1:FK:168:PRO:HD2	1.74	0.69
1:FG:92:PHE:HB2	1:FG:113:MET:HE1	1.74	0.68
1:EJ:212:HIS:HB2	1:EJ:222:PRO:HG3	1.74	0.68
1:EE:166:LYS:HG3	1:EE:168:PRO:HD2	1.74	0.68
1:DC:145:ALA:HB2	1:DC:285:PRO:HD3	1.74	0.68
1:DE:396:ASN:OD1	1:DE:400:ASN:ND2	2.27	0.68
1:GD:283:TYR:HB3	1:GD:307:GLN:HE21	1.59	0.68
1:EF:402:ARG:NE	1:FG:392:ASP:OD2	2.26	0.67
1:DB:145:ALA:HB2	1:DB:285:PRO:HD3	1.76	0.67
1:EA:125:PRO:HG2	1:EA:309:GLN:HB2	1.77	0.67
1:GG:149:THR:HB	1:GG:281:ASN:HD21	1.58	0.67
1:FC:145:ALA:HB2	1:FC:285:PRO:HD3	1.76	0.67
1:DG:237:LEU:HD21	1:DG:241:GLY:H	1.57	0.67
1:DJ:46:LYS:HB2	1:EK:56:ILE:HD12	1.76	0.67
1:EJ:293:ILE:HG12	1:EJ:299:VAL:HG12	1.76	0.67
1:GH:145:ALA:HB2	1:GH:285:PRO:HD3	1.76	0.67
1:DA:145:ALA:HB2	1:DA:285:PRO:HD3	1.76	0.67
1:DE:158:ASN:ND2	1:DE:269:ASN:O	2.27	0.66
1:DB:94:SER:HB2	1:DB:332:VAL:HG12	1.77	0.66
1:EB:179:LYS:HD2	1:EB:273:ASN:HB3	1.78	0.66
1:EC:145:ALA:HB2	1:EC:285:PRO:HD3	1.76	0.66
1:FD:145:ALA:HB2	1:FD:285:PRO:HD3	1.77	0.66
1:DF:101:LEU:HD21	1:DF:138:ILE:HD12	1.77	0.66
1:DI:94:SER:HB2	1:DI:332:VAL:HG12	1.78	0.66
1:GA:177:TYR:HA	1:GA:200:VAL:HG12	1.78	0.66
1:GF:92:PHE:HB2	1:GF:113:MET:HE1	1.78	0.66
1:GI:145:ALA:HB2	1:GI:285:PRO:HD3	1.76	0.66
1:DH:145:ALA:HB2	1:DH:285:PRO:HD3	1.78	0.65
1:GG:83:ARG:HD2	1:GG:344:LEU:HD11	1.76	0.65
1:FK:230:LYS:HB2	1:FK:239:SER:HB3	1.76	0.65
1:DH:351:ASN:ND2	1:EI:288:LEU:O	2.29	0.65
1:FI:145:ALA:HB2	1:FI:285:PRO:HD3	1.78	0.65
1:DK:177:TYR:HA	1:DK:200:VAL:HG22	1.77	0.65
1:GC:70:ARG:NH2	1:GC:99:PHE:O	2.27	0.65
1:EC:161:ASP:OD2	1:EC:178:ASN:ND2	2.30	0.65
1:EF:106:ASN:HB3	1:EF:137:THR:HG22	1.79	0.64
1:FJ:212:HIS:HB2	1:FJ:222:PRO:HG3	1.80	0.64
1:EF:94:SER:HB2	1:EF:332:VAL:HG12	1.79	0.64
1:EH:402:ARG:HD2	1:FH:375:ILE:HG12	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FA:125:PRO:HG2	1:FA:309:GLN:HB2	1.79	0.64
1:GF:94:SER:HB3	1:GF:332:VAL:HG12	1.80	0.64
1:DD:94:SER:HB2	1:DD:332:VAL:HG12	1.79	0.64
1:DG:155:ILE:HG13	1:DG:275:ILE:HA	1.80	0.64
1:FF:18:VAL:O	1:FF:22:ASN:ND2	2.31	0.64
1:DF:145:ALA:HB2	1:DF:285:PRO:HD3	1.79	0.64
1:EH:145:ALA:HB2	1:EH:285:PRO:HD3	1.78	0.64
1:DH:230:LYS:HB2	1:DH:239:SER:HB3	1.80	0.63
1:FE:145:ALA:HB2	1:FE:285:PRO:HD3	1.78	0.63
1:GE:94:SER:HB2	1:GE:332:VAL:HG12	1.80	0.63
1:DK:366:ASP:OD2	1:DK:369:LYS:NZ	2.32	0.63
1:EH:106:ASN:HB3	1:EH:137:THR:HG22	1.80	0.63
1:EF:177:TYR:HA	1:EF:200:VAL:HG12	1.79	0.63
1:FJ:105:ARG:NH1	1:FJ:138:ILE:O	2.31	0.63
1:EE:70:ARG:NH2	1:EE:99:PHE:O	2.32	0.63
1:DG:180:LYS:HE2	1:DG:196:ASN:HD21	1.63	0.63
1:EK:402:ARG:NH2	1:FK:378:GLN:OE1	2.31	0.63
1:EK:198:TYR:HB2	1:EK:210:TYR:HB2	1.80	0.63
1:GB:31:PHE:HB3	1:GB:363:SER:HB2	1.81	0.63
1:GD:325:LEU:HD13	1:GD:333:TRP:HB3	1.81	0.62
1:GH:61:THR:O	1:GH:364:ASN:ND2	2.32	0.62
1:GI:117:GLY:HA2	1:GI:315:VAL:HG23	1.81	0.62
1:DF:106:ASN:HB3	1:DF:137:THR:HG22	1.81	0.62
1:EK:249:THR:OG1	1:EK:253:ALA:O	2.15	0.62
1:FH:106:ASN:HB3	1:FH:137:THR:HG22	1.81	0.62
1:FG:251:ASN:O	1:FG:251:ASN:ND2	2.25	0.62
1:EB:159:SER:HA	1:EB:267:GLN:HE21	1.65	0.62
1:EC:32:LYS:NZ	1:EC:361:GLU:OE2	2.33	0.62
1:GH:157:LEU:HD13	1:GH:207:TRP:CE2	2.34	0.62
1:EI:94:SER:HB2	1:EI:332:VAL:HG12	1.80	0.62
1:GJ:127:ILE:HG21	1:GJ:313:GLN:HE21	1.65	0.62
1:GJ:212:HIS:HB2	1:GJ:222:PRO:HG3	1.80	0.62
1:DF:72:LEU:HD21	1:DF:291:TYR:HE2	1.64	0.62
1:DG:177:TYR:HA	1:DG:200:VAL:HG12	1.80	0.62
1:EB:94:SER:HB2	1:EB:332:VAL:HG12	1.80	0.62
1:EC:49:LEU:HB3	1:FC:64:THR:HG22	1.82	0.62
1:DH:154:GLN:NE2	1:DH:264:ASN:O	2.30	0.61
1:FA:145:ALA:HB2	1:FA:285:PRO:HD3	1.82	0.61
1:FB:177:TYR:HA	1:FB:200:VAL:HG12	1.81	0.61
1:GH:115:LEU:HD21	1:GH:314:ILE:HD12	1.82	0.61
1:DG:402:ARG:HH11	1:EG:375:ILE:HG12	1.65	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FF:161:ASP:OD2	1:FF:178:ASN:ND2	2.33	0.61
1:FH:161:ASP:OD2	1:FH:178:ASN:ND2	2.33	0.61
1:GJ:229:LEU:HD22	1:GJ:237:LEU:HD11	1.82	0.61
1:DE:128:GLN:OE1	1:EE:180:LYS:NZ	2.32	0.61
1:EA:3:SER:HB2	1:FA:64:THR:HG21	1.82	0.61
1:EE:125:PRO:HG2	1:EE:309:GLN:HG3	1.83	0.61
1:DC:94:SER:HB2	1:DC:332:VAL:HG12	1.81	0.61
1:DH:70:ARG:NH2	1:DH:99:PHE:O	2.34	0.61
1:EB:177:TYR:HA	1:EB:200:VAL:HG12	1.83	0.61
1:DD:145:ALA:HB2	1:DD:285:PRO:HD3	1.82	0.61
1:DE:177:TYR:HA	1:DE:200:VAL:HG22	1.81	0.61
1:GJ:11:ALA:HB1	1:GJ:38:PHE:HE1	1.64	0.61
1:GJ:211:THR:HG21	1:GJ:245:ILE:HG21	1.83	0.61
1:DH:4:GLN:NE2	1:EI:17:ASP:OD1	2.33	0.61
1:FK:86:ASP:OD1	1:FK:87:SER:N	2.34	0.61
1:GJ:169:PHE:HA	1:GJ:176:SER:HB3	1.82	0.61
1:FH:402:ARG:HH11	1:GH:375:ILE:HG12	1.66	0.61
1:GA:123:THR:OG1	1:GA:124:PRO:HD3	2.01	0.61
1:GB:145:ALA:HB2	1:GB:285:PRO:HD3	1.83	0.61
1:EA:143:MET:HE3	1:EA:305:ASN:HD21	1.66	0.61
1:EJ:143:MET:HE1	1:EJ:307:GLN:HB2	1.81	0.61
1:FC:402:ARG:NH2	1:GA:386:GLN:OE1	2.34	0.61
1:FJ:399:VAL:O	1:GI:386:GLN:NE2	2.34	0.61
1:ED:42:PHE:HB2	1:FE:329:GLY:HA2	1.83	0.60
1:EJ:145:ALA:HB2	1:EJ:285:PRO:HD3	1.82	0.60
1:FG:284:LYS:O	1:FG:305:ASN:ND2	2.34	0.60
1:FH:145:ALA:HB2	1:FH:285:PRO:HD3	1.82	0.60
1:DE:158:ASN:ND2	1:DE:271:GLY:O	2.34	0.60
1:DG:145:ALA:HB2	1:DG:285:PRO:HD3	1.84	0.60
1:GA:145:ALA:HB2	1:GA:285:PRO:HD3	1.83	0.60
1:DK:166:LYS:HG3	1:DK:168:PRO:HD2	1.82	0.60
1:GK:229:LEU:HD22	1:GK:237:LEU:HD11	1.82	0.60
1:DC:70:ARG:NH2	1:DC:99:PHE:O	2.33	0.60
1:DH:209:VAL:O	1:DH:226:SER:OG	2.18	0.60
1:GJ:117:GLY:HA2	1:GJ:315:VAL:HG13	1.83	0.60
1:GJ:227:THR:HG21	1:GJ:243:VAL:HG11	1.82	0.60
1:DA:246:THR:HB	1:DA:257:THR:HG23	1.84	0.60
1:GD:177:TYR:HA	1:GD:200:VAL:HG12	1.83	0.60
1:EI:143:MET:HE1	1:EI:307:GLN:HB2	1.83	0.60
1:EK:177:TYR:HA	1:EK:200:VAL:HG12	1.84	0.60
1:FD:86:ASP:OD1	1:FD:87:SER:N	2.35	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FC:295:ASN:OD1	1:FC:357:ASN:ND2	2.35	0.60
1:ED:145:ALA:HB2	1:ED:285:PRO:HD3	1.81	0.60
1:GC:32:LYS:NZ	1:GC:361:GLU:OE2	2.34	0.60
1:FH:70:ARG:NH2	1:FH:99:PHE:O	2.34	0.60
1:FH:101:LEU:HD21	1:FH:138:ILE:HD12	1.82	0.60
1:FJ:396:ASN:O	1:FJ:400:ASN:ND2	2.34	0.60
1:GH:291:TYR:HA	1:GH:301:GLY:HA2	1.84	0.60
1:GJ:18:VAL:O	1:GJ:22:ASN:ND2	2.34	0.60
1:EH:7:SER:OG	1:EH:51:VAL:O	2.19	0.59
1:DI:177:TYR:HA	1:DI:200:VAL:HG22	1.83	0.59
1:GE:161:ASP:OD1	1:GE:178:ASN:ND2	2.35	0.59
1:DE:156:ASN:HD22	1:DE:157:LEU:N	2.00	0.59
1:EC:3:SER:HB3	1:FC:64:THR:HG21	1.85	0.59
1:GE:123:THR:OG1	1:GE:124:PRO:HD3	2.02	0.59
1:DJ:166:LYS:NZ	1:DJ:173:ASP:OD2	2.36	0.59
1:EH:70:ARG:NH2	1:EH:99:PHE:O	2.33	0.59
1:GH:184:THR:O	1:GH:280:GLN:NE2	2.35	0.59
1:EB:188:SER:OG	1:FK:234:ASN:OD1	2.19	0.59
1:EF:145:ALA:HB2	1:EF:285:PRO:HD3	1.84	0.59
1:FA:94:SER:HB2	1:FA:332:VAL:HG12	1.84	0.59
1:FD:293:ILE:O	1:FD:357:ASN:ND2	2.33	0.59
1:DC:295:ASN:OD1	1:DC:357:ASN:ND2	2.35	0.59
1:DH:94:SER:HB3	1:DH:332:VAL:HG12	1.85	0.59
1:FK:143:MET:HE1	1:FK:307:GLN:HB2	1.84	0.59
1:GF:379:ARG:HG3	1:GG:395:LEU:HB3	1.85	0.59
1:DG:371:LEU:HA	1:DG:374:MET:HE3	1.84	0.59
1:EE:49:LEU:HD22	1:FE:64:THR:HG23	1.85	0.59
1:EJ:316:LEU:HD11	1:EJ:355:LEU:HD11	1.84	0.59
1:DJ:159:SER:HA	1:DJ:267:GLN:HE21	1.67	0.58
1:DE:123:THR:OG1	1:DE:124:PRO:HD3	2.02	0.58
1:FC:379:ARG:NH1	1:FC:382:GLN:OE1	2.37	0.58
1:EI:70:ARG:NH2	1:EI:99:PHE:O	2.35	0.58
1:GA:125:PRO:HG2	1:GA:309:GLN:HG3	1.84	0.58
1:GF:98:GLN:HB3	1:GF:110:MET:HE3	1.85	0.58
1:GG:139:PRO:HB2	1:GG:141:THR:HG23	1.83	0.58
1:GK:166:LYS:NZ	1:GK:173:ASP:OD1	2.36	0.58
1:DG:207:TRP:HB2	1:DG:229:LEU:HB2	1.86	0.58
1:ED:101:LEU:HD21	1:ED:138:ILE:HD12	1.83	0.58
1:FA:187:ASP:OD1	1:FA:191:ASN:N	2.34	0.58
1:GD:197:VAL:HG12	1:GD:211:THR:HG22	1.85	0.58
1:EF:70:ARG:NH2	1:EF:99:PHE:O	2.37	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EJ:229:LEU:HD22	1:EJ:237:LEU:HD11	1.85	0.58
1:FE:86:ASP:OD1	1:FE:87:SER:N	2.36	0.58
1:EA:195:MET:HE1	1:EA:258:PHE:HZ	1.67	0.58
1:EC:207:TRP:O	1:EC:229:LEU:N	2.37	0.58
1:FI:303:TYR:HE2	1:FI:309:GLN:HB2	1.69	0.58
1:GA:379:ARG:NH1	1:GA:382:GLN:OE1	2.37	0.58
1:EH:230:LYS:HB2	1:EH:239:SER:HB2	1.85	0.58
1:EJ:398:LEU:HD21	1:FJ:368:SER:HA	1.86	0.58
1:GD:23:ILE:HD11	1:GD:370:GLU:HB2	1.86	0.58
1:DJ:68:THR:HG21	1:DJ:360:LEU:HD12	1.86	0.58
1:EK:79:ASN:HB3	1:EK:318:ASN:HD21	1.69	0.58
1:GD:354:LYS:HD3	1:GD:355:LEU:H	1.68	0.58
1:FD:70:ARG:NH1	1:FD:98:GLN:OE1	2.37	0.57
1:GJ:298:THR:HG22	1:GJ:313:GLN:HB2	1.86	0.57
1:EH:117:GLY:HA2	1:EH:315:VAL:HG12	1.86	0.57
1:FG:251:ASN:HD22	1:FG:251:ASN:C	2.12	0.57
1:FA:101:LEU:HD21	1:FA:138:ILE:HD12	1.86	0.57
1:GA:94:SER:HB2	1:GA:332:VAL:HG12	1.86	0.57
1:GG:177:TYR:HA	1:GG:200:VAL:HG12	1.86	0.57
1:DE:146:LYS:NZ	1:DE:281:ASN:O	2.37	0.57
1:FH:293:ILE:O	1:FH:357:ASN:ND2	2.37	0.57
1:EE:123:THR:OG1	1:EE:124:PRO:HD3	2.03	0.57
1:FG:43:ALA:HB2	1:FG:49:LEU:HD11	1.85	0.57
1:GD:161:ASP:O	1:GD:201:LYS:NZ	2.37	0.57
1:DK:70:ARG:NH2	1:DK:99:PHE:O	2.38	0.57
1:EA:187:ASP:OD1	1:EA:191:ASN:N	2.37	0.57
1:EG:70:ARG:NH2	1:EG:99:PHE:O	2.38	0.57
1:FD:159:SER:O	1:FE:251:ASN:ND2	2.37	0.57
1:GJ:94:SER:HB3	1:GJ:332:VAL:HG12	1.86	0.57
1:EA:235:GLY:HA2	1:EA:267:GLN:HB3	1.87	0.57
1:FG:401:LEU:HD12	1:FH:389:LYS:HE3	1.87	0.57
1:GB:400:ASN:OD1	1:GB:401:LEU:N	2.38	0.57
1:DH:402:ARG:NH2	1:EH:378:GLN:OE1	2.38	0.57
1:GH:187:ASP:OD2	1:GH:193:HIS:NE2	2.35	0.56
1:DD:212:HIS:HB2	1:DD:222:PRO:HG3	1.87	0.56
1:DE:284:LYS:O	1:DE:305:ASN:ND2	2.29	0.56
1:DK:203:LYS:HB3	1:DK:206:GLU:HG3	1.85	0.56
1:EC:187:ASP:OD1	1:EC:191:ASN:N	2.39	0.56
1:EH:57:THR:HG21	1:FI:110:MET:HE1	1.88	0.56
1:FB:145:ALA:HB2	1:FB:285:PRO:HD3	1.86	0.56
1:FJ:187:ASP:HA	1:FJ:256:ALA:HB2	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GI:316:LEU:HB2	1:GI:352:PHE:HD1	1.70	0.56
1:DE:70:ARG:NH2	1:DE:99:PHE:O	2.39	0.56
1:ED:247:THR:OG1	1:ED:256:ALA:N	2.38	0.56
1:FF:145:ALA:HB2	1:FF:285:PRO:HD3	1.86	0.56
1:FI:1:SER:OG	1:FI:2:PHE:N	2.39	0.56
1:GE:86:ASP:OD1	1:GE:87:SER:N	2.39	0.56
1:DI:143:MET:HE1	1:DI:307:GLN:HB2	1.87	0.56
1:EB:196:ASN:OD1	1:EB:214:SER:OG	2.23	0.56
1:FA:379:ARG:NH1	1:FA:382:GLN:OE1	2.39	0.56
1:EA:49:LEU:HB3	1:FA:64:THR:HG22	1.88	0.56
1:EE:284:LYS:O	1:EE:305:ASN:ND2	2.28	0.56
1:GC:94:SER:HB2	1:GC:332:VAL:HG12	1.88	0.56
1:FF:201:LYS:NZ	1:FF:204:ASP:O	2.39	0.56
1:EJ:76:ILE:HB	1:EJ:95:ARG:HH21	1.71	0.56
1:DJ:229:LEU:HD22	1:DJ:237:LEU:HD11	1.86	0.56
1:FE:70:ARG:NH2	1:FE:99:PHE:O	2.39	0.56
1:DK:149:THR:HG22	1:DK:281:ASN:HD21	1.71	0.56
1:EB:254:THR:HG23	1:FK:233:GLU:HG3	1.87	0.56
1:FK:184:THR:O	1:FK:280:GLN:NE2	2.39	0.56
1:DF:83:ARG:HD2	1:DF:344:LEU:HD11	1.87	0.55
1:EE:232:ASN:OD1	1:EE:233:GLU:N	2.38	0.55
1:FG:177:TYR:HA	1:FG:200:VAL:HG12	1.87	0.55
1:DB:177:TYR:HA	1:DB:200:VAL:HG12	1.88	0.55
1:EF:166:LYS:HG2	1:EF:168:PRO:HD2	1.88	0.55
1:EI:210:TYR:HE2	1:EI:225:ALA:HA	1.71	0.55
1:FB:379:ARG:NH1	1:FB:382:GLN:OE1	2.39	0.55
1:FC:94:SER:HB2	1:FC:332:VAL:HG12	1.88	0.55
1:FD:169:PHE:HA	1:FD:176:SER:HB3	1.88	0.55
1:DK:229:LEU:HD11	1:DK:237:LEU:HD11	1.87	0.55
1:EJ:128:GLN:HE21	1:EJ:131:ALA:HB2	1.71	0.55
1:DA:187:ASP:OD1	1:DA:191:ASN:N	2.40	0.55
1:GB:203:LYS:NZ	1:GB:206:GLU:OE1	2.34	0.55
1:GH:76:ILE:HB	1:GH:95:ARG:HH21	1.70	0.55
1:DC:68:THR:HG21	1:DC:360:LEU:HD12	1.87	0.55
1:FG:145:ALA:HB2	1:FG:285:PRO:HD3	1.89	0.55
1:DB:187:ASP:OD1	1:DB:191:ASN:N	2.40	0.55
1:DG:123:THR:HG23	1:DG:124:PRO:HD3	1.89	0.55
1:FF:86:ASP:OD1	1:FF:87:SER:N	2.40	0.55
1:GF:318:ASN:ND2	1:GF:351:ASN:OD1	2.39	0.55
1:EF:399:VAL:HG11	1:FE:382:GLN:HB3	1.88	0.55
1:EK:74:VAL:HG12	1:EK:357:ASN:HA	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FD:394:ILE:HD11	1:GE:378:GLN:HG3	1.89	0.55
1:FF:207:TRP:NE1	1:FF:267:GLN:OE1	2.39	0.55
1:GB:298:THR:HG22	1:GB:313:GLN:HG3	1.89	0.55
1:GI:125:PRO:HG3	1:GI:309:GLN:HG3	1.88	0.55
1:DA:158:ASN:ND2	1:DA:271:GLY:O	2.40	0.55
1:DA:261:SER:HB3	1:DA:263:LEU:HD13	1.88	0.55
1:DC:230:LYS:HD2	1:DC:239:SER:HB3	1.89	0.55
1:EJ:402:ARG:HH22	1:FJ:374:MET:HE3	1.72	0.55
1:EK:152:SER:HB3	1:EK:279:ASN:HB3	1.89	0.55
1:EB:379:ARG:NH1	1:EB:382:GLN:OE1	2.39	0.55
1:FJ:32:LYS:NZ	1:FJ:361:GLU:OE2	2.39	0.55
1:FJ:205:ASN:OD1	1:FJ:267:GLN:NE2	2.40	0.55
1:FK:203:LYS:HG2	1:FK:204:ASP:H	1.72	0.55
1:FK:229:LEU:HD22	1:FK:237:LEU:HD11	1.88	0.55
1:GH:77:SER:OG	1:GH:354:LYS:N	2.38	0.55
1:DE:398:LEU:HD21	1:EE:368:SER:HA	1.89	0.54
1:DG:152:SER:OG	1:DG:279:ASN:OD1	2.16	0.54
1:GD:123:THR:OG1	1:GD:124:PRO:HD2	2.07	0.54
1:GD:295:ASN:OD1	1:GD:296:ASP:N	2.40	0.54
1:GJ:137:THR:HG23	1:GJ:139:PRO:HD3	1.87	0.54
1:FH:143:MET:HE3	1:FH:309:GLN:HG3	1.87	0.54
1:GH:370:GLU:HA	1:GH:373:ASN:HB2	1.90	0.54
1:EA:123:THR:OG1	1:EA:124:PRO:HD3	2.08	0.54
1:EF:230:LYS:HE2	1:EF:239:SER:HB3	1.88	0.54
1:FG:280:GLN:OE1	1:FG:282:GLY:N	2.39	0.54
1:GF:30:GLY:N	1:GF:361:GLU:O	2.35	0.54
1:EA:303:TYR:OH	1:EA:309:GLN:NE2	2.39	0.54
1:EJ:68:THR:HG21	1:EJ:360:LEU:HD12	1.89	0.54
1:FA:1:SER:N	1:GA:366:ASP:OD1	2.39	0.54
1:GD:159:SER:OG	1:GD:267:GLN:O	2.26	0.54
1:EB:9:LEU:HD22	1:EB:384:ASN:HB3	1.89	0.54
1:EG:125:PRO:HG2	1:EG:309:GLN:HG3	1.90	0.54
1:EG:145:ALA:HB2	1:EG:285:PRO:HD3	1.89	0.54
1:EG:41:MET:HE1	1:FG:67:ASN:HD22	1.72	0.54
1:GC:145:ALA:HB2	1:GC:285:PRO:HD3	1.88	0.54
1:GE:198:TYR:HB2	1:GE:210:TYR:HB2	1.89	0.54
1:DE:170:SER:HB3	1:DE:173:ASP:HB2	1.89	0.54
1:FD:94:SER:HB2	1:FD:332:VAL:HG12	1.89	0.54
1:GE:46:LYS:HB3	1:GF:56:ILE:HD12	1.90	0.54
1:DE:156:ASN:HD22	1:DE:157:LEU:H	1.56	0.54
1:DG:246:THR:HG22	1:DG:257:THR:HG22	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EF:158:ASN:ND2	1:EF:271:GLY:O	2.41	0.54
1:FI:105:ARG:NH1	1:FI:138:ILE:O	2.40	0.54
1:GC:296:ASP:OD2	1:GC:313:GLN:NE2	2.41	0.54
1:GE:401:LEU:HA	1:GF:389:LYS:HE2	1.88	0.54
1:GB:33:SER:HB3	1:GB:365:VAL:HG22	1.89	0.54
1:GG:121:THR:OG1	1:GG:128:GLN:OE1	2.26	0.54
1:GG:232:ASN:HD22	1:GG:236:ILE:HB	1.73	0.54
1:DA:185:VAL:HG23	1:DA:193:HIS:HB2	1.90	0.53
1:DH:155:ILE:HG12	1:DH:199:PHE:HE1	1.72	0.53
1:ED:293:ILE:O	1:ED:357:ASN:ND2	2.41	0.53
1:GD:207:TRP:HB2	1:GD:229:LEU:HB2	1.89	0.53
1:GE:379:ARG:NH1	1:GE:382:GLN:OE1	2.40	0.53
1:EA:166:LYS:HZ3	1:EA:168:PRO:HG2	1.73	0.53
1:EH:143:MET:HG3	1:EH:309:GLN:NE2	2.23	0.53
1:GD:195:MET:HE3	1:GD:195:MET:HA	1.91	0.53
1:EK:70:ARG:NH2	1:EK:99:PHE:O	2.35	0.53
1:DA:156:ASN:HB3	1:DA:266:MET:HE2	1.89	0.53
1:DB:32:LYS:NZ	1:DB:361:GLU:OE2	2.41	0.53
1:DJ:148:THR:HG21	1:DJ:185:VAL:HB	1.91	0.53
1:EB:145:ALA:HB2	1:EB:285:PRO:HD3	1.91	0.53
1:EC:379:ARG:NH1	1:EC:382:GLN:OE1	2.41	0.53
1:FF:149:THR:HG1	1:FF:281:ASN:HD21	1.55	0.53
1:GK:165:SER:OG	1:GK:175:ASP:OD2	2.27	0.53
1:FJ:46:LYS:HB2	1:GK:56:ILE:HD12	1.90	0.53
1:GD:92:PHE:HB3	1:GD:332:VAL:HB	1.90	0.53
1:GD:120:ALA:HB1	1:GD:125:PRO:HB2	1.91	0.53
1:GF:21:ASN:OD1	1:GF:25:ASN:ND2	2.42	0.53
1:EA:68:THR:HG21	1:EA:360:LEU:HD12	1.89	0.53
1:EC:317:ALA:HB2	1:EC:344:LEU:HD23	1.89	0.53
1:EE:146:LYS:NZ	1:EE:281:ASN:O	2.41	0.53
1:FB:166:LYS:NZ	1:FB:168:PRO:HG2	2.24	0.53
1:FC:261:SER:HB2	1:FC:263:LEU:HD23	1.90	0.53
1:GB:161:ASP:OD2	1:GB:178:ASN:ND2	2.41	0.53
1:GJ:202:THR:OG1	1:GJ:206:GLU:O	2.26	0.53
1:EI:284:LYS:O	1:EI:305:ASN:ND2	2.35	0.53
1:FD:402:ARG:NH2	1:GD:378:GLN:OE1	2.42	0.53
1:GJ:233:GLU:OE2	1:GK:254:THR:OG1	2.26	0.53
1:GI:108:VAL:HG12	1:GI:114:GLN:HA	1.91	0.53
1:EH:236:ILE:HG22	1:EH:266:MET:HE3	1.90	0.53
1:GE:125:PRO:HG2	1:GE:309:GLN:HG3	1.90	0.53
1:FI:143:MET:HE1	1:FI:307:GLN:HB2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GB:62:ASP:OD2	1:GB:63:GLY:N	2.42	0.52
1:GE:68:THR:HG21	1:GE:360:LEU:HD12	1.91	0.52
1:GF:80:GLY:HA3	1:GF:316:LEU:HD13	1.90	0.52
1:GH:292:GLN:NE2	1:GH:294:ASN:OD1	2.41	0.52
1:DJ:145:ALA:HB2	1:DJ:285:PRO:HD3	1.91	0.52
1:EF:401:LEU:HD21	1:FG:388:ILE:HG21	1.90	0.52
1:EJ:49:LEU:HD22	1:FJ:64:THR:HG23	1.90	0.52
1:FA:166:LYS:NZ	1:FA:168:PRO:O	2.38	0.52
1:FH:106:ASN:HA	1:FH:137:THR:HA	1.91	0.52
1:FJ:187:ASP:OD1	1:FJ:191:ASN:N	2.42	0.52
1:GD:155:ILE:HG21	1:GD:199:PHE:HE2	1.75	0.52
1:GA:68:THR:HG21	1:GA:360:LEU:HD12	1.91	0.52
1:FB:161:ASP:OD2	1:FB:178:ASN:ND2	2.43	0.52
1:GA:43:ALA:HB2	1:GA:49:LEU:HD11	1.92	0.52
1:GJ:93:TYR:O	1:GJ:333:TRP:N	2.33	0.52
1:GJ:159:SER:HA	1:GJ:267:GLN:HE21	1.75	0.52
1:DF:73:ASP:O	1:DF:358:GLY:N	2.41	0.52
1:EC:190:GLY:O	1:FA:269:ASN:ND2	2.37	0.52
1:EJ:284:LYS:O	1:EJ:305:ASN:ND2	2.31	0.52
1:FF:396:ASN:OD1	1:FF:400:ASN:ND2	2.42	0.52
1:GI:380:ASN:O	1:GI:384:ASN:ND2	2.37	0.52
1:DE:179:LYS:HB2	1:DE:273:ASN:HD22	1.74	0.52
1:DJ:231:PHE:HE1	1:DJ:237:LEU:HD12	1.74	0.52
1:ED:177:TYR:HA	1:ED:200:VAL:HG12	1.92	0.52
1:FD:177:TYR:HA	1:FD:200:VAL:HG12	1.90	0.52
1:FF:102:ASP:OD1	1:FF:103:GLU:N	2.43	0.52
1:GJ:123:THR:HB	1:GJ:124:PRO:HD3	1.91	0.52
1:EJ:249:THR:OG1	1:EJ:253:ALA:O	2.25	0.52
1:EK:49:LEU:HD13	1:FK:64:THR:HG22	1.91	0.52
1:GI:293:ILE:O	1:GI:357:ASN:ND2	2.42	0.52
1:EK:390:THR:O	1:EK:394:ILE:HG12	2.10	0.52
1:FB:196:ASN:OD1	1:FB:214:SER:OG	2.28	0.52
1:GA:108:VAL:HG12	1:GA:114:GLN:HA	1.92	0.52
1:GB:21:ASN:O	1:GB:25:ASN:ND2	2.40	0.52
1:GC:379:ARG:NH1	1:GC:382:GLN:OE1	2.38	0.52
1:GF:179:LYS:HD2	1:GF:180:LYS:N	2.24	0.52
1:DA:143:MET:SD	1:DA:305:ASN:ND2	2.77	0.52
1:DI:145:ALA:HB2	1:DI:285:PRO:HD3	1.91	0.52
1:DI:212:HIS:HB2	1:DI:222:PRO:HG3	1.92	0.52
1:DI:235:GLY:HA2	1:DI:266:MET:HE1	1.91	0.52
1:GD:205:ASN:ND2	1:GD:232:ASN:O	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GH:106:ASN:HB3	1:GH:137:THR:HG22	1.92	0.52
1:FK:167:THR:OG1	1:FK:168:PRO:HD3	2.10	0.51
1:GB:379:ARG:NH1	1:GB:382:GLN:OE1	2.43	0.51
1:GH:213:ASP:OD2	1:GH:247:THR:OG1	2.24	0.51
1:GH:290:SER:O	1:GH:302:ASN:N	2.43	0.51
1:GH:386:GLN:HA	1:GH:389:LYS:HD2	1.92	0.51
1:EI:123:THR:HB	1:EI:124:PRO:HD3	1.91	0.51
1:FF:198:TYR:HB2	1:FF:210:TYR:HB2	1.93	0.51
1:FI:290:SER:OG	1:FI:302:ASN:OD1	2.28	0.51
1:GB:211:THR:HG21	1:GB:245:ILE:HG21	1.90	0.51
1:GG:145:ALA:HB2	1:GG:285:PRO:HD3	1.92	0.51
1:DG:15:ASN:O	1:DG:19:ILE:HG12	2.10	0.51
1:DI:187:ASP:OD1	1:DI:191:ASN:N	2.44	0.51
1:FJ:148:THR:HG21	1:FJ:185:VAL:HB	1.90	0.51
1:GA:247:THR:HG22	1:GA:256:ALA:H	1.74	0.51
1:DH:201:LYS:HD3	1:DH:207:TRP:CE2	2.45	0.51
1:DB:158:ASN:HD21	1:DB:161:ASP:HB2	1.76	0.51
1:DK:94:SER:HB2	1:DK:332:VAL:HG12	1.93	0.51
1:FF:169:PHE:HE2	1:FF:222:PRO:HG2	1.76	0.51
1:FG:166:LYS:HG2	1:FG:168:PRO:HD2	1.92	0.51
1:FG:393:GLN:OE1	1:FH:378:GLN:NE2	2.40	0.51
1:FH:226:SER:HB3	1:FH:243:VAL:HG11	1.92	0.51
1:GC:177:TYR:HA	1:GC:200:VAL:HG12	1.91	0.51
1:DC:185:VAL:HG22	1:DC:195:MET:HE1	1.93	0.51
1:DC:285:PRO:HG3	1:EA:268:GLN:HB3	1.93	0.51
1:DE:210:TYR:HE2	1:DE:225:ALA:HA	1.76	0.51
1:DI:70:ARG:NH2	1:DI:99:PHE:O	2.43	0.51
1:EB:303:TYR:HE1	1:EB:309:GLN:HB2	1.76	0.51
1:EK:212:HIS:HB2	1:EK:222:PRO:HG3	1.92	0.51
1:FD:396:ASN:HD22	1:GC:379:ARG:HH22	1.59	0.51
1:FI:187:ASP:HA	1:FI:256:ALA:HB2	1.92	0.51
1:GA:207:TRP:NE1	1:GA:267:GLN:OE1	2.41	0.51
1:GC:101:LEU:HD21	1:GC:138:ILE:HD12	1.92	0.51
1:DC:102:ASP:OD1	1:DC:103:GLU:N	2.43	0.51
1:FF:62:ASP:OD2	1:FF:95:ARG:NH2	2.44	0.51
1:FF:284:LYS:O	1:FF:305:ASN:ND2	2.42	0.51
1:GD:145:ALA:HB2	1:GD:285:PRO:HD3	1.91	0.51
1:GH:232:ASN:HD21	1:GH:236:ILE:HG22	1.74	0.51
1:DA:106:ASN:ND2	1:DA:114:GLN:OE1	2.43	0.51
1:FG:207:TRP:NE1	1:FG:267:GLN:OE1	2.43	0.51
1:GH:109:ASN:HD21	1:GH:113:MET:HB2	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FI:68:THR:HG21	1:FI:360:LEU:HD12	1.92	0.51
1:FJ:207:TRP:NE1	1:FJ:267:GLN:OE1	2.28	0.51
1:DB:209:VAL:HB	1:DB:227:THR:HG22	1.93	0.51
1:FH:123:THR:HB	1:FH:124:PRO:HD3	1.93	0.51
1:FK:379:ARG:NH1	1:FK:382:GLN:OE1	2.44	0.51
1:GJ:108:VAL:HG12	1:GJ:114:GLN:HA	1.93	0.51
1:EK:379:ARG:NH1	1:EK:382:GLN:OE1	2.44	0.50
1:FB:34:GLY:HA2	1:FB:58:GLN:HA	1.93	0.50
1:GG:202:THR:OG1	1:GG:206:GLU:OE1	2.26	0.50
1:GH:327:SER:HG	1:GH:333:TRP:CD1	2.30	0.50
1:GI:196:ASN:OD1	1:GI:214:SER:OG	2.29	0.50
1:DA:148:THR:HG21	1:DA:185:VAL:HG12	1.93	0.50
1:DE:207:TRP:NE1	1:DE:267:GLN:OE1	2.45	0.50
1:DH:251:ASN:HD22	1:DH:251:ASN:C	2.19	0.50
1:DH:254:THR:N	1:EG:233:GLU:OE1	2.34	0.50
1:FJ:94:SER:HB2	1:FJ:332:VAL:HG12	1.93	0.50
1:GA:32:LYS:NZ	1:GA:361:GLU:OE2	2.42	0.50
1:DC:210:TYR:CE1	1:DC:225:ALA:HA	2.46	0.50
1:DE:138:ILE:HA	1:DE:311:LEU:HD13	1.91	0.50
1:DI:386:GLN:O	1:DI:390:THR:HG23	2.11	0.50
1:EG:351:ASN:O	1:EG:351:ASN:ND2	2.42	0.50
1:EJ:102:ASP:OD1	1:EJ:103:GLU:N	2.40	0.50
1:FK:187:ASP:OD1	1:FK:191:ASN:N	2.45	0.50
1:FK:249:THR:OG1	1:FK:253:ALA:O	2.24	0.50
1:DA:379:ARG:NH1	1:DA:382:GLN:OE1	2.42	0.50
1:DG:209:VAL:O	1:DG:226:SER:N	2.44	0.50
1:DI:330:ASP:OD1	1:DI:331:ASN:N	2.44	0.50
1:EJ:179:LYS:HD3	1:EJ:273:ASN:HB2	1.93	0.50
1:EF:143:MET:HE1	1:EF:307:GLN:HB2	1.92	0.50
1:GB:211:THR:HG21	1:GB:245:ILE:HD13	1.94	0.50
1:GF:287:ASP:H	1:GF:304:SER:HB3	1.77	0.50
1:GG:92:PHE:HB3	1:GG:332:VAL:HB	1.93	0.50
1:DE:294:ASN:ND2	1:DE:298:THR:OG1	2.43	0.50
1:DJ:201:LYS:HD3	1:DJ:207:TRP:CE2	2.46	0.50
1:EJ:187:ASP:OD1	1:EJ:191:ASN:N	2.44	0.50
1:EK:187:ASP:OD1	1:EK:191:ASN:N	2.45	0.50
1:FI:232:ASN:HD21	1:FI:236:ILE:HB	1.77	0.50
1:EF:284:LYS:O	1:EF:305:ASN:ND2	2.38	0.50
1:FJ:287:ASP:OD1	1:FJ:287:ASP:N	2.45	0.50
1:GE:169:PHE:HA	1:GE:176:SER:HB3	1.92	0.50
1:EI:33:SER:HB3	1:EI:365:VAL:HG22	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FG:179:LYS:NZ	1:FG:273:ASN:O	2.36	0.50
1:GC:198:TYR:HB2	1:GC:210:TYR:HB2	1.93	0.50
1:DG:394:ILE:HD11	1:DH:378:GLN:HA	1.94	0.50
1:EA:199:PHE:HE1	1:EA:262:PHE:HE1	1.60	0.50
1:FA:232:ASN:OD1	1:FA:233:GLU:N	2.36	0.50
1:ED:72:LEU:HD11	1:ED:107:LEU:HD21	1.93	0.49
1:EE:158:ASN:N	1:EE:273:ASN:OD1	2.39	0.49
1:EI:196:ASN:OD1	1:EI:214:SER:OG	2.27	0.49
1:GC:187:ASP:OD2	1:GC:193:HIS:NE2	2.45	0.49
1:GJ:145:ALA:HB2	1:GJ:285:PRO:HG3	1.94	0.49
1:DF:285:PRO:HG2	1:EE:270:THR:H	1.76	0.49
1:DF:316:LEU:HD11	1:DF:355:LEU:HD11	1.94	0.49
1:FE:328:GLN:HB2	1:FE:332:VAL:HG23	1.94	0.49
1:GB:232:ASN:OD1	1:GB:233:GLU:N	2.45	0.49
1:GC:61:THR:O	1:GC:364:ASN:ND2	2.44	0.49
1:GF:117:GLY:HA2	1:GF:315:VAL:HG13	1.94	0.49
1:GG:179:LYS:NZ	1:GG:180:LYS:O	2.44	0.49
1:GG:247:THR:OG1	1:GG:256:ALA:N	2.44	0.49
1:GG:290:SER:HB3	1:GG:302:ASN:HB2	1.94	0.49
1:GJ:230:LYS:HB2	1:GJ:239:SER:HB2	1.94	0.49
1:DF:366:ASP:O	1:DF:370:GLU:HG2	2.12	0.49
1:FC:207:TRP:O	1:FC:229:LEU:N	2.44	0.49
1:GI:154:GLN:HB2	1:GI:276:VAL:HB	1.93	0.49
1:DF:94:SER:HB3	1:DF:332:VAL:HG12	1.93	0.49
1:DF:169:PHE:HA	1:DF:176:SER:HB3	1.94	0.49
1:FB:149:THR:HG1	1:FB:281:ASN:HD21	1.60	0.49
1:FI:94:SER:HB3	1:FI:332:VAL:HG12	1.94	0.49
1:DI:137:THR:HG23	1:DI:139:PRO:HD3	1.94	0.49
1:EE:205:ASN:ND2	1:EE:231:PHE:O	2.45	0.49
1:FI:284:LYS:O	1:FI:305:ASN:ND2	2.40	0.49
1:GB:227:THR:HG21	1:GB:243:VAL:HG21	1.93	0.49
1:GJ:195:MET:HE3	1:GJ:195:MET:HA	1.93	0.49
1:DD:148:THR:HG22	1:DD:282:GLY:HA3	1.95	0.49
1:FF:187:ASP:OD1	1:FF:191:ASN:N	2.46	0.49
1:DB:5:ALA:HB1	1:DB:388:ILE:HG12	1.95	0.49
1:DC:43:ALA:HB1	1:EC:62:ASP:HB2	1.94	0.49
1:DH:169:PHE:HE1	1:DH:177:TYR:HB3	1.78	0.49
1:ED:46:LYS:HB2	1:FE:56:ILE:HD13	1.93	0.49
1:EG:123:THR:HB	1:EG:124:PRO:HD3	1.94	0.49
1:EG:169:PHE:HE2	1:EG:177:TYR:HD2	1.61	0.49
1:GB:393:GLN:HA	1:GB:396:ASN:HB3	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GC:166:LYS:HE2	1:GC:168:PRO:HD2	1.95	0.49
1:GD:370:GLU:HA	1:GD:373:ASN:HB2	1.94	0.49
1:DC:158:ASN:OD1	1:DC:273:ASN:ND2	2.45	0.49
1:DC:300:VAL:HG12	1:DC:310:VAL:HG22	1.95	0.49
1:EF:186:TYR:HE2	1:EF:284:LYS:HE3	1.76	0.49
1:FJ:74:VAL:HG12	1:FJ:357:ASN:HA	1.95	0.49
1:DE:125:PRO:HG2	1:DE:309:GLN:HG3	1.94	0.48
1:DG:402:ARG:NH2	1:EG:378:GLN:OE1	2.45	0.48
1:DI:196:ASN:OD1	1:DI:212:HIS:HB3	2.13	0.48
1:FG:206:GLU:HG2	1:FG:230:LYS:HD2	1.95	0.48
1:FH:120:ALA:HB2	1:FH:127:ILE:HD13	1.96	0.48
1:GB:76:ILE:O	1:GB:95:ARG:NH2	2.46	0.48
1:DI:390:THR:O	1:DI:394:ILE:HG23	2.13	0.48
1:DK:209:VAL:HB	1:DK:227:THR:HB	1.94	0.48
1:FK:155:ILE:O	1:FK:265:SER:OG	2.31	0.48
1:GB:7:SER:OG	1:GB:51:VAL:O	2.32	0.48
1:GI:187:ASP:OD1	1:GI:191:ASN:N	2.45	0.48
1:DC:298:THR:HG22	1:DC:313:GLN:HG3	1.96	0.48
1:DE:139:PRO:HB2	1:DE:141:THR:HG23	1.93	0.48
1:DF:209:VAL:HG23	1:DF:226:SER:HB2	1.96	0.48
1:DK:247:THR:HG22	1:DK:256:ALA:H	1.78	0.48
1:EC:266:MET:HB3	1:EC:268:GLN:OE1	2.13	0.48
1:EG:236:ILE:HD12	1:EG:236:ILE:H	1.78	0.48
1:EK:204:ASP:OD1	1:EK:205:ASN:N	2.46	0.48
1:FB:254:THR:N	1:GK:233:GLU:OE2	2.46	0.48
1:GF:145:ALA:HB2	1:GF:285:PRO:HD3	1.95	0.48
1:EC:147:SER:HB2	1:EC:188:SER:HA	1.95	0.48
1:EH:143:MET:HG3	1:EH:309:GLN:HE21	1.78	0.48
1:EK:108:VAL:HG12	1:EK:114:GLN:HA	1.96	0.48
1:FJ:313:GLN:OE1	1:FJ:346:THR:OG1	2.29	0.48
1:FK:120:ALA:HB2	1:FK:127:ILE:HD13	1.95	0.48
1:GD:73:ASP:HB2	1:GD:360:LEU:HD21	1.95	0.48
1:GG:167:THR:OG1	1:GG:168:PRO:HD3	2.14	0.48
1:GJ:207:TRP:O	1:GJ:229:LEU:N	2.41	0.48
1:DC:290:SER:HG	1:DC:302:ASN:HD22	1.60	0.48
1:EH:379:ARG:HG3	1:EI:395:LEU:HD13	1.95	0.48
1:GC:207:TRP:HE1	1:GC:267:GLN:NE2	2.11	0.48
1:EA:198:TYR:HB2	1:EA:210:TYR:HB2	1.95	0.48
1:EA:263:LEU:HD12	1:EA:264:ASN:H	1.77	0.48
1:EJ:185:VAL:HG23	1:EJ:193:HIS:HB2	1.96	0.48
1:EK:92:PHE:HB3	1:EK:332:VAL:HB	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FF:94:SER:HB3	1:FF:332:VAL:HG12	1.96	0.48
1:FG:149:THR:HB	1:FG:281:ASN:HD21	1.79	0.48
1:FK:187:ASP:HB3	1:FK:193:HIS:NE2	2.29	0.48
1:GI:33:SER:HB3	1:GI:365:VAL:HG22	1.95	0.48
1:DA:179:LYS:HB3	1:DA:199:PHE:HD2	1.79	0.48
1:DF:233:GLU:OE2	1:DG:188:SER:OG	2.31	0.48
1:DJ:1:SER:OG	1:DJ:2:PHE:N	2.47	0.48
1:DJ:154:GLN:OE1	1:DJ:276:VAL:HB	2.14	0.48
1:EC:94:SER:HB2	1:EC:332:VAL:HG12	1.95	0.48
1:GB:187:ASP:OD1	1:GB:191:ASN:N	2.45	0.48
1:DI:209:VAL:O	1:DI:226:SER:HB2	2.13	0.48
1:EC:315:VAL:HG22	1:EC:344:LEU:HD22	1.96	0.48
1:EG:402:ARG:NH2	1:FG:378:GLN:OE1	2.42	0.48
1:EJ:174:ALA:HA	1:EJ:177:TYR:CZ	2.49	0.48
1:GE:76:ILE:HG21	1:GE:80:GLY:HA3	1.93	0.48
1:DJ:263:LEU:HG	1:DJ:264:ASN:OD1	2.14	0.48
1:DK:127:ILE:HD11	1:DK:310:VAL:HG11	1.96	0.48
1:FF:139:PRO:HD2	1:FF:311:LEU:HD22	1.95	0.48
1:FJ:167:THR:OG1	1:FJ:168:PRO:HD3	2.14	0.48
1:FJ:229:LEU:HD22	1:FJ:237:LEU:HD11	1.96	0.48
1:GG:158:ASN:HB3	1:GG:161:ASP:HB2	1.96	0.48
1:DA:79:ASN:OD1	1:DA:318:ASN:ND2	2.47	0.48
1:DE:94:SER:HB2	1:DE:332:VAL:HG12	1.95	0.48
1:DF:382:GLN:HB3	1:DG:399:VAL:HG11	1.96	0.48
1:DH:206:GLU:HB3	1:DH:230:LYS:HD2	1.96	0.48
1:DK:32:LYS:HB2	1:DK:58:GLN:NE2	2.22	0.48
1:EH:123:THR:HB	1:EH:124:PRO:HD3	1.95	0.48
1:GK:107:LEU:HD23	1:GK:115:LEU:HD23	1.95	0.48
1:EG:232:ASN:HD21	1:EG:236:ILE:HD13	1.78	0.47
1:ED:94:SER:HB2	1:ED:332:VAL:HG12	1.96	0.47
1:EG:237:LEU:HD21	1:EG:240:GLY:HA3	1.96	0.47
1:EI:98:GLN:HG2	1:EI:110:MET:HE3	1.96	0.47
1:FJ:207:TRP:O	1:FJ:229:LEU:N	2.37	0.47
1:GB:93:TYR:O	1:GB:333:TRP:N	2.39	0.47
1:GC:193:HIS:HE1	1:GC:250:ILE:HG12	1.78	0.47
1:DC:210:TYR:HE1	1:DC:225:ALA:HA	1.79	0.47
1:DE:300:VAL:HG22	1:DE:310:VAL:HG12	1.96	0.47
1:DJ:212:HIS:HB2	1:DJ:222:PRO:HG3	1.96	0.47
1:EF:287:ASP:H	1:EF:304:SER:HB3	1.79	0.47
1:FE:49:LEU:HD22	1:GE:64:THR:HG23	1.96	0.47
1:GC:148:THR:HG21	1:GC:185:VAL:HG12	1.94	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GF:345:GLY:HA3	1:GF:352:PHE:HE1	1.79	0.47
1:DB:293:ILE:O	1:DB:357:ASN:ND2	2.47	0.47
1:DD:68:THR:HG21	1:DD:360:LEU:HD12	1.97	0.47
1:GD:216:ASP:HB3	1:GD:219:ALA:HB2	1.96	0.47
1:GG:380:ASN:O	1:GG:384:ASN:ND2	2.46	0.47
1:GK:306:GLU:O	1:GK:306:GLU:HG3	2.15	0.47
1:DC:169:PHE:HA	1:DC:176:SER:HB3	1.94	0.47
1:FD:186:TYR:HE2	1:FD:280:GLN:HE22	1.62	0.47
1:FJ:205:ASN:HA	1:FJ:267:GLN:HE22	1.78	0.47
1:GC:185:VAL:HG23	1:GC:193:HIS:HB2	1.97	0.47
1:DG:123:THR:CG2	1:DG:124:PRO:HD3	2.45	0.47
1:EE:197:VAL:HG12	1:EE:211:THR:HG22	1.97	0.47
1:EF:280:GLN:NE2	1:EF:282:GLY:O	2.42	0.47
1:FC:230:LYS:HE2	1:FC:230:LYS:HB3	1.71	0.47
1:FJ:230:LYS:HB2	1:FJ:239:SER:HB2	1.97	0.47
1:FK:158:ASN:OD1	1:FK:270:THR:N	2.39	0.47
1:GA:187:ASP:HA	1:GA:256:ALA:HB2	1.95	0.47
1:GB:389:LYS:O	1:GB:393:GLN:HG3	2.15	0.47
1:GH:211:THR:HG22	1:GH:226:SER:HB2	1.96	0.47
1:DC:378:GLN:O	1:DC:382:GLN:HG3	2.15	0.47
1:DF:287:ASP:OD1	1:DF:288:LEU:N	2.46	0.47
1:DG:206:GLU:HG3	1:DG:230:LYS:NZ	2.29	0.47
1:EA:195:MET:HA	1:EA:213:ASP:HA	1.97	0.47
1:ED:68:THR:HG21	1:ED:360:LEU:HD12	1.96	0.47
1:ED:287:ASP:OD1	1:ED:288:LEU:N	2.47	0.47
1:EH:33:SER:HB3	1:EH:365:VAL:HG22	1.97	0.47
1:FB:29:TYR:O	1:FB:96:ASN:ND2	2.46	0.47
1:FB:285:PRO:HG3	1:GK:268:GLN:HB3	1.96	0.47
1:FC:40:ASP:HB2	1:FD:330:ASP:O	2.15	0.47
1:FD:179:LYS:HD2	1:FD:273:ASN:HB3	1.97	0.47
1:FF:206:GLU:OE1	1:FF:228:THR:OG1	2.23	0.47
1:FI:153:MET:HG3	1:FI:278:THR:HG22	1.96	0.47
1:GE:177:TYR:HA	1:GE:200:VAL:HG12	1.97	0.47
1:GG:40:ASP:HB2	1:GH:330:ASP:O	2.13	0.47
1:GI:316:LEU:HB2	1:GI:352:PHE:CD1	2.50	0.47
1:GJ:11:ALA:HB1	1:GJ:38:PHE:CE1	2.48	0.47
1:DA:1:SER:OG	1:DA:391:GLN:OE1	2.32	0.47
1:DC:209:VAL:O	1:DC:226:SER:HB3	2.15	0.47
1:EA:204:ASP:OD1	1:EA:204:ASP:N	2.47	0.47
1:EF:108:VAL:HG12	1:EF:114:GLN:HA	1.96	0.47
1:FF:1:SER:OG	1:FF:2:PHE:N	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DH:243:VAL:HG23	1:DH:260:LEU:HD21	1.96	0.47
1:EJ:167:THR:OG1	1:EJ:168:PRO:HD3	2.15	0.47
1:EJ:299:VAL:HG23	1:EJ:311:LEU:HB2	1.96	0.47
1:FC:123:THR:HB	1:FC:124:PRO:HD2	1.97	0.47
1:FJ:145:ALA:HB2	1:FJ:285:PRO:HD3	1.96	0.47
1:GF:149:THR:OG1	1:GF:281:ASN:ND2	2.40	0.47
1:GG:230:LYS:H	1:GG:239:SER:HB3	1.80	0.47
1:GH:206:GLU:HG3	1:GH:229:LEU:O	2.15	0.47
1:DE:159:SER:HB3	1:DE:267:GLN:HG2	1.96	0.47
1:DH:366:ASP:O	1:DH:370:GLU:HG2	2.15	0.47
1:DK:29:TYR:O	1:DK:96:ASN:ND2	2.48	0.47
1:EK:203:LYS:HE3	1:EK:206:GLU:HG3	1.96	0.47
1:FE:123:THR:OG1	1:FE:124:PRO:HD2	2.15	0.47
1:GH:157:LEU:HD22	1:GH:207:TRP:CH2	2.49	0.47
1:DB:166:LYS:NZ	1:DB:168:PRO:HG2	2.29	0.46
1:DD:72:LEU:HD23	1:DD:100:LYS:HA	1.96	0.46
1:DH:8:GLY:HA3	1:DH:384:ASN:ND2	2.29	0.46
1:EI:398:LEU:HD21	1:FI:368:SER:HA	1.96	0.46
1:FB:94:SER:HB2	1:FB:332:VAL:HG12	1.97	0.46
1:DI:372:VAL:O	1:DI:376:VAL:HG23	2.15	0.46
1:EK:155:ILE:O	1:EK:265:SER:OG	2.30	0.46
1:FH:149:THR:OG1	1:FH:281:ASN:ND2	2.31	0.46
1:GC:287:ASP:OD1	1:GC:287:ASP:N	2.47	0.46
1:DB:380:ASN:O	1:DB:384:ASN:ND2	2.46	0.46
1:DF:195:MET:HE3	1:DF:195:MET:HB3	1.81	0.46
1:EC:43:ALA:HB1	1:FC:62:ASP:HB2	1.97	0.46
1:EE:402:ARG:NH2	1:FE:378:GLN:OE1	2.49	0.46
1:FE:284:LYS:O	1:FE:305:ASN:ND2	2.48	0.46
1:FG:125:PRO:HG2	1:FG:309:GLN:HG2	1.97	0.46
1:FG:139:PRO:HB2	1:FG:141:THR:HG23	1.96	0.46
1:FI:125:PRO:HG2	1:FI:309:GLN:HG2	1.96	0.46
1:GA:83:ARG:HD2	1:GA:344:LEU:HD21	1.98	0.46
1:DG:50:GLY:O	1:DH:25:ASN:ND2	2.43	0.46
1:EC:149:THR:HB	1:EC:281:ASN:HD21	1.81	0.46
1:EI:155:ILE:O	1:EI:265:SER:OG	2.27	0.46
1:FG:148:THR:HG21	1:FG:185:VAL:HG12	1.97	0.46
1:FI:177:TYR:HA	1:FI:200:VAL:HG22	1.97	0.46
1:FK:177:TYR:HA	1:FK:200:VAL:HG22	1.97	0.46
1:GD:179:LYS:HD2	1:GD:273:ASN:HB3	1.97	0.46
1:GJ:318:ASN:HB2	1:GJ:352:PHE:CE1	2.51	0.46
1:GK:187:ASP:OD1	1:GK:191:ASN:N	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EB:287:ASP:OD2	1:EB:287:ASP:N	2.46	0.46
1:EF:195:MET:HE3	1:EF:195:MET:HB3	1.83	0.46
1:FC:177:TYR:HA	1:FC:200:VAL:HG12	1.97	0.46
1:GB:117:GLY:HA3	1:GB:136:ILE:HD11	1.97	0.46
1:DB:202:THR:OG1	1:DB:206:GLU:OE2	2.31	0.46
1:DB:209:VAL:O	1:DB:226:SER:N	2.48	0.46
1:EA:230:LYS:HA	1:EA:230:LYS:HD3	1.68	0.46
1:EH:198:TYR:HB2	1:EH:210:TYR:HB2	1.98	0.46
1:FA:68:THR:HG21	1:FA:360:LEU:HD12	1.97	0.46
1:GF:74:VAL:O	1:GF:97:GLY:HA3	2.16	0.46
1:GF:261:SER:HB3	1:GF:263:LEU:HD23	1.96	0.46
1:DK:92:PHE:HB2	1:DK:113:MET:HE1	1.98	0.46
1:DK:187:ASP:OD1	1:DK:191:ASN:N	2.46	0.46
1:FA:43:ALA:HB2	1:FA:49:LEU:HD11	1.97	0.46
1:FD:203:LYS:HB2	1:FD:206:GLU:HB2	1.97	0.46
1:FF:153:MET:HE3	1:FF:275:ILE:HD13	1.97	0.46
1:FH:167:THR:HB	1:FH:168:PRO:HD3	1.98	0.46
1:GC:33:SER:OG	1:GC:364:ASN:O	2.31	0.46
1:DK:372:VAL:O	1:DK:376:VAL:HG23	2.15	0.46
1:EH:83:ARG:HH11	1:EH:116:THR:HG21	1.81	0.46
1:EJ:402:ARG:HD3	1:FJ:375:ILE:HG12	1.96	0.46
1:FJ:390:THR:O	1:FJ:394:ILE:HG12	2.16	0.46
1:GI:366:ASP:O	1:GI:370:GLU:HG2	2.16	0.46
1:DC:209:VAL:CG2	1:DC:227:THR:HB	2.46	0.46
1:DF:153:MET:HG2	1:DF:278:THR:HG22	1.98	0.46
1:DJ:305:ASN:O	1:DJ:307:GLN:HG2	2.16	0.46
1:EA:206:GLU:HG3	1:EA:230:LYS:NZ	2.31	0.46
1:EB:204:ASP:OD1	1:EB:204:ASP:N	2.49	0.46
1:GC:166:LYS:HG3	1:GC:168:PRO:HD2	1.98	0.46
1:GC:167:THR:HB	1:GC:168:PRO:HD3	1.97	0.46
1:GF:270:THR:H	1:GG:285:PRO:HG2	1.81	0.46
1:DA:385:ALA:O	1:DA:388:ILE:HG22	2.15	0.46
1:FB:187:ASP:HA	1:FB:256:ALA:HB2	1.97	0.46
1:FF:398:LEU:HG	1:GF:371:LEU:HD12	1.98	0.46
1:GB:208:ALA:HA	1:GB:228:THR:HA	1.98	0.46
1:DD:42:PHE:HB2	1:EE:329:GLY:HA2	1.98	0.45
1:DF:177:TYR:HA	1:DF:200:VAL:HG12	1.99	0.45
1:DI:179:LYS:NZ	1:DI:273:ASN:O	2.39	0.45
1:DJ:210:TYR:CD1	1:DJ:225:ALA:HA	2.51	0.45
1:DK:155:ILE:O	1:DK:265:SER:OG	2.31	0.45
1:FB:107:LEU:HD23	1:FB:107:LEU:HA	1.85	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FB:187:ASP:OD1	1:FB:191:ASN:N	2.48	0.45
1:FH:201:LYS:HD3	1:FH:207:TRP:CE2	2.51	0.45
1:FI:230:LYS:HB2	1:FI:239:SER:HB2	1.98	0.45
1:GK:284:LYS:O	1:GK:305:ASN:ND2	2.46	0.45
1:DK:117:GLY:HA2	1:DK:315:VAL:HG12	1.98	0.45
1:EB:227:THR:HB	1:EB:243:VAL:HG11	1.97	0.45
1:EH:153:MET:HG3	1:EH:278:THR:HG22	1.97	0.45
1:FA:227:THR:HG21	1:FA:243:VAL:HG22	1.99	0.45
1:FH:366:ASP:O	1:FH:370:GLU:HG2	2.15	0.45
1:FJ:120:ALA:HB2	1:FJ:127:ILE:HD13	1.99	0.45
1:GK:179:LYS:HB3	1:GK:199:PHE:HB2	1.98	0.45
1:DA:402:ARG:HD2	1:DA:402:ARG:HA	1.84	0.45
1:EA:195:MET:HE1	1:EA:258:PHE:CZ	2.51	0.45
1:EE:153:MET:HE1	1:EE:181:GLY:HA3	1.98	0.45
1:EF:169:PHE:HA	1:EF:176:SER:HB3	1.97	0.45
1:FC:369:LYS:HE3	1:FC:369:LYS:HB3	1.72	0.45
1:FG:173:ASP:OD2	1:FG:176:SER:N	2.48	0.45
1:GB:4:GLN:NE2	1:GB:48:GLY:O	2.40	0.45
1:GJ:32:LYS:NZ	1:GJ:361:GLU:OE2	2.39	0.45
1:DD:393:GLN:O	1:DD:397:THR:HG23	2.16	0.45
1:ED:296:ASP:N	1:ED:296:ASP:OD1	2.47	0.45
1:GH:123:THR:HB	1:GH:124:PRO:HD3	1.97	0.45
1:DB:72:LEU:HD23	1:DB:100:LYS:HA	1.99	0.45
1:DD:372:VAL:O	1:DD:376:VAL:HG23	2.17	0.45
1:FK:187:ASP:HA	1:FK:256:ALA:HB2	1.98	0.45
1:DE:229:LEU:HD22	1:DE:237:LEU:HD11	1.99	0.45
1:DJ:117:GLY:HA2	1:DJ:315:VAL:HG13	1.98	0.45
1:GF:201:LYS:HB2	1:GF:201:LYS:HE3	1.79	0.45
1:GJ:156:ASN:HD22	1:GK:142:LEU:HD22	1.81	0.45
1:DH:123:THR:HB	1:DH:124:PRO:HD3	1.99	0.45
1:DK:19:ILE:O	1:DK:23:ILE:HG13	2.17	0.45
1:FB:57:THR:HG21	1:GA:110:MET:HE3	1.99	0.45
1:FH:380:ASN:O	1:FH:384:ASN:ND2	2.41	0.45
1:FJ:121:THR:O	1:FJ:128:GLN:NE2	2.42	0.45
1:FK:164:PRO:HG3	1:FK:200:VAL:HG13	1.99	0.45
1:GE:42:PHE:HB2	1:GF:329:GLY:HA2	1.99	0.45
1:GF:143:MET:HE3	1:GF:309:GLN:HB2	1.99	0.45
1:DJ:154:GLN:HB3	1:DJ:277:ALA:HB3	1.99	0.45
1:DJ:389:LYS:O	1:DJ:393:GLN:HG2	2.16	0.45
1:EJ:68:THR:OG1	1:EJ:73:ASP:OD2	2.29	0.45
1:FA:287:ASP:OD1	1:FA:287:ASP:N	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FB:155:ILE:HD12	1:FB:275:ILE:HG13	1.99	0.45
1:GB:328:GLN:HB2	1:GB:332:VAL:HG23	1.99	0.45
1:GB:392:ASP:OD1	1:GB:393:GLN:N	2.49	0.45
1:GF:29:TYR:CG	1:GF:360:LEU:HD23	2.52	0.45
1:DB:329:GLY:HA3	1:DK:42:PHE:H	1.82	0.45
1:DG:196:ASN:ND2	1:DG:198:TYR:OH	2.50	0.45
1:EH:205:ASN:OD1	1:EH:267:GLN:NE2	2.50	0.45
1:EJ:232:ASN:OD1	1:EJ:236:ILE:N	2.46	0.45
1:EK:101:LEU:HG	1:EK:105:ARG:HA	1.98	0.45
1:DC:384:ASN:O	1:DC:388:ILE:HG12	2.17	0.45
1:DK:261:SER:HB3	1:DK:263:LEU:HD13	1.99	0.45
1:EB:70:ARG:O	1:EB:358:GLY:HA2	2.17	0.45
1:EH:233:GLU:O	1:EI:189:GLN:NE2	2.39	0.45
1:EJ:198:TYR:O	1:EJ:209:VAL:HA	2.17	0.45
1:FC:187:ASP:OD1	1:FC:191:ASN:N	2.48	0.45
1:FI:159:SER:HA	1:FI:267:GLN:HE21	1.82	0.45
1:GB:94:SER:HB3	1:GB:332:VAL:HG12	1.99	0.45
1:DC:366:ASP:O	1:DC:370:GLU:HG2	2.17	0.44
1:DI:379:ARG:HA	1:DI:379:ARG:HD3	1.83	0.44
1:FG:251:ASN:ND2	1:FG:251:ASN:C	2.73	0.44
1:DA:84:LEU:HB2	1:DA:113:MET:HE2	2.00	0.44
1:DA:123:THR:OG1	1:DA:124:PRO:HD2	2.18	0.44
1:DI:123:THR:HB	1:DI:124:PRO:HD3	1.99	0.44
1:EG:398:LEU:HD11	1:FG:368:SER:HA	1.98	0.44
1:FH:83:ARG:HH21	1:FH:116:THR:HG21	1.83	0.44
1:FI:101:LEU:HD21	1:FI:138:ILE:HD12	1.99	0.44
1:GF:200:VAL:O	1:GF:208:ALA:N	2.43	0.44
1:GG:187:ASP:HA	1:GG:256:ALA:HB2	1.98	0.44
1:DD:169:PHE:HE2	1:DD:177:TYR:HB3	1.81	0.44
1:DI:138:ILE:HA	1:DI:311:LEU:HD23	1.99	0.44
1:DI:155:ILE:HG21	1:DI:199:PHE:HE2	1.82	0.44
1:EC:179:LYS:HB2	1:EC:273:ASN:HD21	1.83	0.44
1:FI:237:LEU:HD12	1:FI:238:GLU:N	2.32	0.44
1:GB:204:ASP:OD1	1:GB:204:ASP:N	2.49	0.44
1:DC:254:THR:OG1	1:EA:233:GLU:OE1	2.36	0.44
1:DF:401:LEU:HD21	1:EG:388:ILE:HG21	1.99	0.44
1:DG:143:MET:HG3	1:DG:309:GLN:NE2	2.33	0.44
1:EA:161:ASP:OD2	1:EA:178:ASN:ND2	2.50	0.44
1:EB:328:GLN:HB2	1:EB:332:VAL:HG23	1.98	0.44
1:EC:290:SER:HG	1:EC:302:ASN:HD22	1.58	0.44
1:ED:70:ARG:NH2	1:ED:99:PHE:O	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EG:250:ILE:HG22	1:EG:251:ASN:OD1	2.17	0.44
1:FC:179:LYS:HD2	1:FC:273:ASN:HB3	1.98	0.44
1:FG:293:ILE:O	1:FG:357:ASN:ND2	2.51	0.44
1:GI:313:GLN:OE1	1:GI:346:THR:OG1	2.29	0.44
1:DB:378:GLN:O	1:DB:382:GLN:HG3	2.17	0.44
1:DI:232:ASN:HD21	1:DI:236:ILE:HB	1.83	0.44
1:DI:305:ASN:O	1:DI:307:GLN:NE2	2.49	0.44
1:EA:146:LYS:NZ	1:EA:281:ASN:O	2.39	0.44
1:EE:74:VAL:HG12	1:EE:357:ASN:HA	1.98	0.44
1:FB:390:THR:O	1:FB:394:ILE:HG12	2.17	0.44
1:FD:166:LYS:HB3	1:FD:166:LYS:HE3	1.73	0.44
1:GH:33:SER:HB2	1:GH:365:VAL:HG22	1.99	0.44
1:GH:161:ASP:O	1:GH:201:LYS:HD2	2.17	0.44
1:GH:283:TYR:CG	1:GH:307:GLN:HG3	2.52	0.44
1:DE:49:LEU:HD22	1:EE:64:THR:HG23	1.99	0.44
1:DH:15:ASN:O	1:DH:19:ILE:HG12	2.17	0.44
1:EB:363:SER:O	1:EB:365:VAL:HG23	2.18	0.44
1:EH:1:SER:OG	1:EH:2:PHE:N	2.51	0.44
1:FE:125:PRO:HG2	1:FE:309:GLN:HG2	2.00	0.44
1:FG:94:SER:OG	1:FG:95:ARG:N	2.51	0.44
1:FH:354:LYS:HB3	1:FH:354:LYS:HE2	1.67	0.44
1:FK:366:ASP:OD2	1:FK:368:SER:OG	2.32	0.44
1:DC:185:VAL:CG2	1:DC:195:MET:HE1	2.47	0.44
1:DD:123:THR:OG1	1:DD:124:PRO:HD2	2.18	0.44
1:DJ:398:LEU:HD21	1:EJ:368:SER:HA	1.98	0.44
1:FF:41:MET:HB2	1:FF:49:LEU:HB2	1.99	0.44
1:FI:68:THR:OG1	1:FI:73:ASP:OD2	2.29	0.44
1:FI:316:LEU:HD11	1:FI:355:LEU:HD11	2.00	0.44
1:GA:70:ARG:HB2	1:GA:73:ASP:OD2	2.17	0.44
1:GH:129:GLN:OE1	1:GH:129:GLN:N	2.48	0.44
1:DC:155:ILE:HD12	1:DC:275:ILE:HA	1.99	0.44
1:DC:246:THR:HG23	1:DC:257:THR:HG22	2.00	0.44
1:DD:187:ASP:OD1	1:DD:191:ASN:N	2.50	0.44
1:DG:399:VAL:HG12	1:DG:400:ASN:H	1.82	0.44
1:DH:187:ASP:OD1	1:DH:191:ASN:N	2.51	0.44
1:DH:199:PHE:CD2	1:DH:209:VAL:HG12	2.52	0.44
1:DK:238:GLU:N	1:DK:238:GLU:OE1	2.51	0.44
1:ED:266:MET:HE3	1:ED:268:GLN:HG3	1.99	0.44
1:GB:363:SER:O	1:GB:365:VAL:HG23	2.18	0.44
1:GG:230:LYS:HB2	1:GG:239:SER:HB3	2.00	0.44
1:DI:210:TYR:CE2	1:DI:225:ALA:HA	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:ED:5:ALA:HB1	1:ED:388:ILE:HG12	1.99	0.44
1:EK:379:ARG:HA	1:EK:379:ARG:HD3	1.83	0.44
1:FE:73:ASP:OD1	1:FE:359:ALA:N	2.51	0.44
1:FG:94:SER:HB2	1:FG:332:VAL:HG12	2.00	0.44
1:FJ:125:PRO:HG2	1:FJ:309:GLN:HG3	1.99	0.44
1:DC:199:PHE:CD1	1:DC:209:VAL:HG12	2.53	0.43
1:ED:285:PRO:HG2	1:FC:270:THR:H	1.83	0.43
1:EF:379:ARG:HG3	1:EG:395:LEU:HD13	1.98	0.43
1:EH:187:ASP:OD1	1:EH:191:ASN:N	2.51	0.43
1:EJ:200:VAL:HG23	1:EJ:202:THR:HG23	1.98	0.43
1:GF:159:SER:N	1:GF:268:GLN:O	2.46	0.43
1:GG:390:THR:O	1:GG:394:ILE:HG12	2.18	0.43
1:DG:68:THR:HG21	1:DG:360:LEU:HD12	2.01	0.43
1:EC:213:ASP:OD2	1:EC:247:THR:OG1	2.37	0.43
1:FA:1:SER:O	1:FA:1:SER:OG	2.34	0.43
1:FA:203:LYS:HG2	1:FA:204:ASP:N	2.32	0.43
1:GB:9:LEU:HD12	1:GB:384:ASN:HB3	1.99	0.43
1:GC:40:ASP:HB2	1:GD:330:ASP:O	2.18	0.43
1:GC:120:ALA:HB1	1:GC:125:PRO:HB3	1.99	0.43
1:GJ:203:LYS:HG3	1:GJ:204:ASP:H	1.83	0.43
1:DA:231:PHE:CZ	1:DA:265:SER:HB2	2.53	0.43
1:DH:251:ASN:O	1:DH:251:ASN:ND2	2.51	0.43
1:EB:143:MET:HE1	1:EB:307:GLN:HB2	2.01	0.43
1:EC:198:TYR:O	1:EC:209:VAL:HA	2.18	0.43
1:FJ:73:ASP:OD1	1:FJ:73:ASP:N	2.52	0.43
1:GF:177:TYR:CE2	1:GF:180:LYS:HB2	2.53	0.43
1:DC:9:LEU:HD11	1:DC:388:ILE:HG13	1.99	0.43
1:DE:390:THR:HG21	1:DF:374:MET:HG2	2.00	0.43
1:DF:202:THR:O	1:DF:206:GLU:HB2	2.18	0.43
1:EI:153:MET:HE3	1:EI:275:ILE:HD12	1.99	0.43
1:FF:111:GLN:HG2	1:FF:330:ASP:HB3	2.01	0.43
1:GF:308:GLU:OE1	1:GF:308:GLU:N	2.51	0.43
1:DJ:378:GLN:O	1:DJ:382:GLN:HG3	2.19	0.43
1:DK:213:ASP:OD2	1:DK:247:THR:OG1	2.36	0.43
1:EF:269:ASN:ND2	1:EG:284:LYS:HE3	2.34	0.43
1:FE:336:THR:HG22	1:FE:338:ALA:H	1.81	0.43
1:FJ:52:LYS:HD2	1:GJ:67:ASN:HD21	1.83	0.43
1:FJ:197:VAL:HA	1:FJ:210:TYR:O	2.19	0.43
1:GA:363:SER:O	1:GA:365:VAL:HG23	2.17	0.43
1:GK:4:GLN:NE2	1:GK:48:GLY:O	2.45	0.43
1:DF:70:ARG:O	1:DF:358:GLY:HA2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EE:180:LYS:HB3	1:EE:180:LYS:HE2	1.70	0.43
1:GD:72:LEU:HD21	1:GD:291:TYR:HE2	1.84	0.43
1:GF:41:MET:HE1	1:GF:43:ALA:HB2	1.99	0.43
1:GH:229:LEU:HD11	1:GH:262:PHE:HD2	1.83	0.43
1:DC:178:ASN:N	1:DC:199:PHE:O	2.52	0.43
1:DG:163:VAL:HG22	1:DG:201:LYS:HG2	2.01	0.43
1:EH:247:THR:OG1	1:EH:256:ALA:N	2.44	0.43
1:EH:366:ASP:O	1:EH:370:GLU:HG2	2.19	0.43
1:EI:187:ASP:OD1	1:EI:191:ASN:N	2.51	0.43
1:EK:149:THR:OG1	1:EK:281:ASN:ND2	2.40	0.43
1:FH:157:LEU:HD13	1:FH:207:TRP:CD2	2.54	0.43
1:GA:98:GLN:HG2	1:GA:110:MET:HE2	2.00	0.43
1:GG:375:ILE:O	1:GG:379:ARG:HG2	2.18	0.43
1:DA:247:THR:OG1	1:DA:248:GLY:N	2.51	0.43
1:DC:154:GLN:HG3	1:DC:263:LEU:O	2.18	0.43
1:DD:46:LYS:HB2	1:EE:56:ILE:HD13	2.01	0.43
1:DD:330:ASP:O	1:DD:331:ASN:ND2	2.51	0.43
1:DE:328:GLN:HB2	1:DE:332:VAL:HG23	1.99	0.43
1:EF:186:TYR:CE2	1:EF:284:LYS:HE3	2.54	0.43
1:EJ:201:LYS:HD3	1:EJ:207:TRP:CZ2	2.54	0.43
1:FF:57:THR:HG21	1:GG:110:MET:HE1	2.00	0.43
1:FF:285:PRO:HG3	1:GE:268:GLN:HB3	2.01	0.43
1:GA:147:SER:HB2	1:GA:188:SER:HA	2.01	0.43
1:GG:123:THR:CG2	1:GG:124:PRO:HD3	2.48	0.43
1:GJ:187:ASP:OD1	1:GJ:191:ASN:N	2.51	0.43
1:DA:380:ASN:O	1:DA:384:ASN:ND2	2.52	0.43
1:DJ:14:THR:O	1:DJ:18:VAL:HG23	2.19	0.43
1:EH:143:MET:HE1	1:EH:307:GLN:HB3	1.99	0.43
1:EI:143:MET:HE3	1:EI:283:TYR:CE1	2.54	0.43
1:FF:154:GLN:HG2	1:FF:276:VAL:HB	2.00	0.43
1:GB:379:ARG:HA	1:GB:379:ARG:HD3	1.71	0.43
1:DF:242:THR:OG1	1:DF:259:SER:OG	2.37	0.43
1:DG:399:VAL:HG12	1:DG:400:ASN:N	2.33	0.43
1:EI:210:TYR:CE2	1:EI:225:ALA:HA	2.52	0.43
1:EK:230:LYS:HB3	1:EK:239:SER:HB2	2.01	0.43
1:FI:33:SER:HB3	1:FI:365:VAL:HG22	2.01	0.43
1:GD:32:LYS:HA	1:GD:32:LYS:HD3	1.74	0.43
1:GH:295:ASN:OD1	1:GH:296:ASP:N	2.52	0.43
1:DC:84:LEU:HD23	1:DC:115:LEU:HA	2.01	0.42
1:DD:72:LEU:HD12	1:DD:72:LEU:HA	1.93	0.42
1:DF:169:PHE:HE1	1:DF:177:TYR:HB3	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DH:260:LEU:HD23	1:DH:260:LEU:H	1.84	0.42
1:DJ:372:VAL:O	1:DJ:376:VAL:HG23	2.18	0.42
1:EC:232:ASN:OD1	1:EC:235:GLY:N	2.46	0.42
1:EC:290:SER:HG	1:EC:302:ASN:ND2	2.14	0.42
1:EE:266:MET:HE3	1:EE:266:MET:HB2	1.88	0.42
1:EE:328:GLN:HB2	1:EE:332:VAL:HG23	2.01	0.42
1:FA:202:THR:OG1	1:FA:206:GLU:OE2	2.32	0.42
1:FE:124:PRO:HA	1:FE:125:PRO:HD3	1.88	0.42
1:FF:268:GLN:HB3	1:FG:285:PRO:HG3	2.00	0.42
1:GH:297:GLY:O	1:GH:314:ILE:HG22	2.19	0.42
1:DA:249:THR:HG22	1:DA:255:ALA:H	1.83	0.42
1:DK:32:LYS:HB3	1:DK:59:ASP:O	2.20	0.42
1:EA:195:MET:HG2	1:EA:213:ASP:HB3	2.01	0.42
1:EB:68:THR:HG23	1:EB:70:ARG:H	1.84	0.42
1:FC:379:ARG:HA	1:FC:379:ARG:HD3	1.80	0.42
1:FE:107:LEU:HD23	1:FE:107:LEU:HA	1.87	0.42
1:FG:306:GLU:OE1	1:FG:306:GLU:N	2.53	0.42
1:FI:196:ASN:OD1	1:FI:214:SER:OG	2.28	0.42
1:GA:402:ARG:HD2	1:GA:402:ARG:HA	1.85	0.42
1:GC:158:ASN:OD1	1:GC:161:ASP:HB2	2.19	0.42
1:GE:49:LEU:HD23	1:GE:49:LEU:HA	1.90	0.42
1:GK:161:ASP:CG	1:GK:178:ASN:HD21	2.27	0.42
1:DD:146:LYS:HB2	1:DD:146:LYS:HE3	1.84	0.42
1:DF:197:VAL:HG22	1:DF:211:THR:HG22	2.00	0.42
1:DF:199:PHE:CD1	1:DF:209:VAL:HG12	2.54	0.42
1:EA:169:PHE:HA	1:EA:176:SER:OG	2.19	0.42
1:EB:381:TYR:CE1	1:EK:394:ILE:HG23	2.54	0.42
1:EE:153:MET:HG2	1:EE:155:ILE:HD11	2.00	0.42
1:EH:84:LEU:HD23	1:EH:115:LEU:HA	2.00	0.42
1:EJ:33:SER:HB3	1:EJ:365:VAL:HG22	2.00	0.42
1:FA:167:THR:HB	1:FA:168:PRO:HD3	2.00	0.42
1:FB:366:ASP:O	1:FB:370:GLU:HG2	2.19	0.42
1:FB:379:ARG:HD3	1:FB:379:ARG:HA	1.88	0.42
1:FC:149:THR:OG1	1:FC:281:ASN:ND2	2.48	0.42
1:FF:125:PRO:HG2	1:FF:309:GLN:HB2	2.00	0.42
1:FI:237:LEU:HD12	1:FI:238:GLU:H	1.84	0.42
1:FK:390:THR:O	1:FK:394:ILE:HG12	2.20	0.42
1:GD:86:ASP:OD1	1:GD:87:SER:N	2.45	0.42
1:GJ:366:ASP:O	1:GJ:370:GLU:HG2	2.19	0.42
1:DB:31:PHE:HB3	1:DB:363:SER:HB2	2.00	0.42
1:DC:264:ASN:O	1:DC:264:ASN:ND2	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DE:161:ASP:O	1:DE:201:LYS:HE2	2.19	0.42
1:DJ:122:GLY:HA2	1:DJ:125:PRO:HA	2.00	0.42
1:DK:379:ARG:HA	1:DK:379:ARG:HD3	1.81	0.42
1:EG:284:LYS:O	1:EG:305:ASN:ND2	2.52	0.42
1:EK:200:VAL:HG23	1:EK:208:ALA:HB3	2.01	0.42
1:FF:81:PHE:HB3	1:FF:93:TYR:HB3	2.00	0.42
1:FG:124:PRO:HA	1:FG:125:PRO:HD3	1.87	0.42
1:FK:203:LYS:HB3	1:FK:206:GLU:HG2	2.01	0.42
1:GH:229:LEU:HD11	1:GH:262:PHE:CD2	2.53	0.42
1:GI:402:ARG:NH1	1:GJ:392:ASP:OD2	2.53	0.42
1:DA:191:ASN:OD1	1:DA:192:ALA:N	2.52	0.42
1:DD:124:PRO:HA	1:DD:125:PRO:HD3	1.96	0.42
1:DF:402:ARG:NH1	1:EF:378:GLN:OE1	2.52	0.42
1:EB:28:THR:O	1:EB:363:SER:HB3	2.19	0.42
1:EB:94:SER:OG	1:EB:95:ARG:N	2.52	0.42
1:EC:324:GLY:O	1:EC:336:THR:OG1	2.38	0.42
1:EG:161:ASP:OD2	1:EG:178:ASN:ND2	2.52	0.42
1:EH:161:ASP:OD2	1:EH:178:ASN:ND2	2.53	0.42
1:EI:125:PRO:HB2	1:EI:310:VAL:HG22	2.00	0.42
1:FG:187:ASP:HA	1:FG:256:ALA:HB2	2.01	0.42
1:GB:143:MET:SD	1:GB:309:GLN:NE2	2.90	0.42
1:GF:394:ILE:O	1:GF:398:LEU:HD23	2.19	0.42
1:GG:185:VAL:HG23	1:GG:193:HIS:HB2	2.01	0.42
1:GI:94:SER:HB2	1:GI:332:VAL:HG12	2.00	0.42
1:GJ:161:ASP:O	1:GJ:201:LYS:NZ	2.45	0.42
1:DC:200:VAL:HG22	1:DC:208:ALA:HB3	2.02	0.42
1:DI:132:ASN:OD1	1:DI:133:PRO:HD2	2.19	0.42
1:EB:183:VAL:HG23	1:EB:195:MET:HB2	2.02	0.42
1:EB:236:ILE:HD12	1:EB:236:ILE:H	1.84	0.42
1:EI:159:SER:HA	1:EI:267:GLN:HE21	1.84	0.42
1:EI:366:ASP:O	1:EI:370:GLU:HG2	2.19	0.42
1:EJ:161:ASP:O	1:EJ:201:LYS:NZ	2.53	0.42
1:EJ:166:LYS:HB3	1:EJ:166:LYS:HE3	1.81	0.42
1:FA:380:ASN:O	1:FA:384:ASN:ND2	2.49	0.42
1:FA:398:LEU:HD21	1:GA:372:VAL:HG23	2.01	0.42
1:GF:195:MET:SD	1:GF:247:THR:HG22	2.60	0.42
1:GH:161:ASP:HB3	1:GH:201:LYS:HE2	2.02	0.42
1:DC:129:GLN:HA	1:DC:129:GLN:OE1	2.20	0.42
1:DD:166:LYS:HG3	1:DD:168:PRO:HD2	2.01	0.42
1:EH:76:ILE:HB	1:EH:95:ARG:HH21	1.83	0.42
1:EK:345:GLY:HA3	1:EK:352:PHE:CE2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FC:92:PHE:HB3	1:FC:332:VAL:HB	2.01	0.42
1:FI:155:ILE:O	1:FI:265:SER:OG	2.33	0.42
1:FI:367:LEU:HD23	1:FI:367:LEU:HA	1.91	0.42
1:FJ:72:LEU:HD23	1:FJ:72:LEU:HA	1.90	0.42
1:FJ:195:MET:HE2	1:FJ:195:MET:HA	2.01	0.42
1:GG:111:GLN:HG3	1:GG:330:ASP:HB3	2.01	0.42
1:GH:167:THR:HB	1:GH:168:PRO:HD3	2.02	0.42
1:DC:153:MET:HE3	1:DC:155:ILE:HD13	2.01	0.42
1:DC:379:ARG:HA	1:DC:379:ARG:HD3	1.71	0.42
1:DE:305:ASN:O	1:DE:307:GLN:HG2	2.20	0.42
1:DF:167:THR:OG1	1:DF:168:PRO:HD3	2.19	0.42
1:ED:179:LYS:HD2	1:ED:273:ASN:HB3	2.00	0.42
1:EI:402:ARG:NH1	1:FI:378:GLN:OE1	2.53	0.42
1:EK:315:VAL:HG21	1:EK:344:LEU:HD23	2.02	0.42
1:FG:390:THR:O	1:FG:394:ILE:HG12	2.18	0.42
1:FI:247:THR:OG1	1:FI:248:GLY:N	2.52	0.42
1:FJ:345:GLY:HA3	1:FJ:352:PHE:CE2	2.55	0.42
1:GD:268:GLN:HE22	1:GE:145:ALA:H	1.66	0.42
1:GD:279:ASN:OD1	1:GD:280:GLN:N	2.53	0.42
1:GG:74:VAL:HG11	1:GG:355:LEU:HD23	2.01	0.42
1:DA:247:THR:HG23	1:DA:255:ALA:HB1	2.02	0.42
1:DD:167:THR:HB	1:DD:168:PRO:HD3	2.02	0.42
1:DE:145:ALA:HB2	1:DE:285:PRO:HD3	2.02	0.42
1:DE:169:PHE:HD1	1:DE:176:SER:HB3	1.84	0.42
1:EE:324:GLY:O	1:EE:336:THR:OG1	2.38	0.42
1:EF:393:GLN:OE1	1:FG:378:GLN:NE2	2.48	0.42
1:EH:170:SER:HB3	1:EH:173:ASP:HB3	2.02	0.42
1:EI:117:GLY:HA2	1:EI:315:VAL:HG12	2.01	0.42
1:EJ:73:ASP:OD1	1:EJ:73:ASP:N	2.53	0.42
1:FC:120:ALA:HB1	1:FC:125:PRO:HB3	2.01	0.42
1:FH:92:PHE:HB3	1:FH:332:VAL:HB	2.01	0.42
1:GB:230:LYS:HD2	1:GB:230:LYS:HA	1.85	0.42
1:GF:33:SER:N	1:GF:364:ASN:OD1	2.53	0.42
1:GF:101:LEU:HD23	1:GF:101:LEU:HA	1.92	0.42
1:DB:379:ARG:HD3	1:DB:379:ARG:HA	1.87	0.42
1:DF:280:GLN:CD	1:DF:282:GLY:H	2.28	0.42
1:DH:8:GLY:HA3	1:DH:384:ASN:HD22	1.84	0.42
1:DK:33:SER:HB3	1:DK:365:VAL:HG22	2.02	0.42
1:DK:101:LEU:HG	1:DK:105:ARG:HA	2.01	0.42
1:ED:40:ASP:OD1	1:ED:40:ASP:N	2.53	0.42
1:EF:72:LEU:HD23	1:EF:72:LEU:HA	1.93	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EG:169:PHE:HE1	1:EG:222:PRO:HG2	1.84	0.42
1:FB:153:MET:HE2	1:FB:275:ILE:HG12	2.02	0.42
1:FF:130:GLY:HA3	1:GF:180:LYS:HD3	2.02	0.42
1:FJ:367:LEU:HD23	1:FJ:367:LEU:HA	1.92	0.42
1:GC:211:THR:HG21	1:GC:245:ILE:HD13	2.02	0.42
1:GF:40:ASP:N	1:GF:40:ASP:OD1	2.52	0.42
1:DA:296:ASP:N	1:DA:296:ASP:OD1	2.50	0.41
1:DB:203:LYS:HD2	1:DB:204:ASP:O	2.19	0.41
1:EE:232:ASN:HB3	1:EE:236:ILE:H	1.83	0.41
1:EE:247:THR:HG23	1:EE:256:ALA:O	2.20	0.41
1:FA:201:LYS:HB2	1:FA:207:TRP:CE3	2.55	0.41
1:FD:73:ASP:OD1	1:FD:73:ASP:N	2.53	0.41
1:FI:402:ARG:NH1	1:FJ:392:ASP:OD1	2.53	0.41
1:FJ:153:MET:HG3	1:FJ:278:THR:HG22	2.02	0.41
1:GE:45:SER:OG	1:GE:46:LYS:N	2.53	0.41
1:GE:185:VAL:HG23	1:GE:193:HIS:HB2	2.03	0.41
1:GH:373:ASN:HA	1:GH:376:VAL:HG22	2.02	0.41
1:GJ:125:PRO:HG2	1:GJ:309:GLN:HB2	2.01	0.41
1:DC:268:GLN:HG3	1:DC:269:ASN:H	1.85	0.41
1:DD:67:ASN:OD1	1:DD:68:THR:N	2.53	0.41
1:ED:187:ASP:OD1	1:ED:191:ASN:N	2.51	0.41
1:EH:221:ALA:HA	1:EH:222:PRO:HD3	1.92	0.41
1:EH:398:LEU:HD11	1:FH:368:SER:HA	2.03	0.41
1:EI:305:ASN:O	1:EI:307:GLN:HG2	2.20	0.41
1:EJ:59:ASP:OD1	1:EJ:61:THR:HG23	2.21	0.41
1:FF:402:ARG:NH2	1:GE:390:THR:OG1	2.53	0.41
1:FK:154:GLN:HG2	1:FK:276:VAL:HB	2.02	0.41
1:GC:32:LYS:HA	1:GC:32:LYS:HD3	1.86	0.41
1:GH:64:THR:O	1:GH:362:ALA:N	2.52	0.41
1:DG:158:ASN:N	1:DG:273:ASN:OD1	2.44	0.41
1:DJ:5:ALA:HB1	1:DJ:388:ILE:HG13	2.01	0.41
1:EI:108:VAL:HG12	1:EI:114:GLN:HG2	2.02	0.41
1:EJ:213:ASP:OD2	1:EJ:247:THR:OG1	2.38	0.41
1:EJ:367:LEU:HD23	1:EJ:367:LEU:HA	1.91	0.41
1:FE:113:MET:HE1	1:FE:332:VAL:HG21	2.01	0.41
1:DE:210:TYR:CE2	1:DE:225:ALA:HA	2.55	0.41
1:DG:153:MET:HG3	1:DG:278:THR:HB	2.01	0.41
1:DK:232:ASN:OD1	1:DK:236:ILE:N	2.48	0.41
1:EB:187:ASP:OD1	1:EB:191:ASN:N	2.52	0.41
1:EI:232:ASN:HB3	1:EI:238:GLU:OE2	2.20	0.41
1:FK:34:GLY:HA2	1:FK:58:GLN:HA	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FK:366:ASP:O	1:FK:370:GLU:HG2	2.21	0.41
1:DB:366:ASP:O	1:DB:370:GLU:HG2	2.21	0.41
1:DE:179:LYS:HB3	1:DE:199:PHE:HB2	2.03	0.41
1:FF:208:ALA:HA	1:FF:228:THR:HA	2.02	0.41
1:FK:179:LYS:HB3	1:FK:199:PHE:HB2	2.03	0.41
1:GA:179:LYS:HB3	1:GA:199:PHE:HB2	2.03	0.41
1:GE:323:GLU:OE2	1:GF:70:ARG:NH2	2.53	0.41
1:DG:201:LYS:HB2	1:DG:207:TRP:HZ3	1.86	0.41
1:DI:102:ASP:OD1	1:DI:103:GLU:N	2.54	0.41
1:DK:207:TRP:NE1	1:DK:267:GLN:OE1	2.46	0.41
1:EC:230:LYS:NZ	1:EC:238:GLU:HG2	2.36	0.41
1:EI:296:ASP:OD1	1:EI:296:ASP:N	2.54	0.41
1:EK:100:LYS:NZ	1:EK:109:ASN:O	2.54	0.41
1:FA:158:ASN:O	1:FA:159:SER:HB3	2.21	0.41
1:FH:402:ARG:NH2	1:GH:378:GLN:OE1	2.54	0.41
1:FI:366:ASP:O	1:FI:370:GLU:HG2	2.21	0.41
1:GC:101:LEU:HD23	1:GC:101:LEU:HA	1.88	0.41
1:DC:117:GLY:HA2	1:DC:315:VAL:HG12	2.01	0.41
1:DG:397:THR:HG21	1:DH:382:GLN:HG2	2.02	0.41
1:EB:280:GLN:OE1	1:EB:282:GLY:N	2.46	0.41
1:EJ:110:MET:HE3	1:EJ:110:MET:HB3	1.81	0.41
1:FB:247:THR:OG1	1:FB:248:GLY:N	2.53	0.41
1:FC:94:SER:OG	1:FC:95:ARG:N	2.53	0.41
1:FD:390:THR:O	1:FD:394:ILE:HG12	2.20	0.41
1:FE:110:MET:HE3	1:FE:110:MET:HB3	1.93	0.41
1:FJ:199:PHE:HB3	1:FJ:207:TRP:CE3	2.55	0.41
1:FJ:199:PHE:HB3	1:FJ:207:TRP:HE3	1.86	0.41
1:GB:41:MET:HG2	1:GB:52:LYS:HE2	2.02	0.41
1:GB:94:SER:HB2	1:GB:331:ASN:O	2.21	0.41
1:GB:161:ASP:O	1:GB:201:LYS:NZ	2.37	0.41
1:GK:379:ARG:HA	1:GK:379:ARG:HD3	1.92	0.41
1:DA:394:ILE:HD13	1:DA:394:ILE:HA	1.90	0.41
1:DB:287:ASP:H	1:DB:304:SER:HG	1.68	0.41
1:DE:70:ARG:O	1:DE:358:GLY:HA2	2.20	0.41
1:DJ:94:SER:OG	1:DJ:95:ARG:N	2.54	0.41
1:EB:203:LYS:HD2	1:EB:204:ASP:O	2.20	0.41
1:EG:193:HIS:CE1	1:EG:250:ILE:HD12	2.55	0.41
1:EI:230:LYS:O	1:EI:237:LEU:HA	2.21	0.41
1:FA:166:LYS:HG2	1:FA:168:PRO:HD2	2.03	0.41
1:FD:107:LEU:HD23	1:FD:107:LEU:HA	1.83	0.41
1:FI:395:LEU:HD23	1:FI:395:LEU:HA	1.93	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GB:329:GLY:HA2	1:GK:42:PHE:HD2	1.85	0.41
1:GG:123:THR:HG23	1:GG:124:PRO:HD3	2.02	0.41
1:GG:371:LEU:HA	1:GG:374:MET:HE3	2.01	0.41
1:GI:125:PRO:HB2	1:GI:310:VAL:HG22	2.02	0.41
1:DA:187:ASP:HB2	1:DA:254:THR:O	2.20	0.41
1:DA:284:LYS:HB2	1:DA:285:PRO:HD2	2.02	0.41
1:DK:123:THR:HA	1:DK:124:PRO:HA	1.85	0.41
1:EC:266:MET:HE2	1:EC:266:MET:HA	2.03	0.41
1:EC:318:ASN:ND2	1:EC:352:PHE:CE2	2.89	0.41
1:ED:344:LEU:HD12	1:ED:344:LEU:H	1.86	0.41
1:EK:260:LEU:HD12	1:EK:261:SER:H	1.85	0.41
1:FA:101:LEU:HD23	1:FA:101:LEU:HA	1.88	0.41
1:FA:366:ASP:O	1:FA:370:GLU:HG2	2.21	0.41
1:FC:209:VAL:HG22	1:FC:227:THR:O	2.21	0.41
1:FD:46:LYS:HB2	1:GE:56:ILE:HD13	2.02	0.41
1:FJ:80:GLY:O	1:FJ:95:ARG:NH1	2.54	0.41
1:FJ:157:LEU:HD13	1:FJ:207:TRP:CE2	2.55	0.41
1:GA:293:ILE:O	1:GA:357:ASN:ND2	2.54	0.41
1:GC:330:ASP:O	1:GC:331:ASN:ND2	2.54	0.41
1:GD:107:LEU:HD23	1:GD:107:LEU:HA	1.95	0.41
1:GE:86:ASP:HB2	1:GE:92:PHE:HE2	1.86	0.41
1:GH:105:ARG:NH2	1:GH:138:ILE:O	2.54	0.41
1:GH:216:ASP:HB3	1:GH:219:ALA:HB2	2.02	0.41
1:DD:177:TYR:CE2	1:DD:180:LYS:HB2	2.55	0.41
1:DE:398:LEU:HD12	1:DE:398:LEU:HA	1.95	0.41
1:DH:189:GLN:NE2	1:EG:233:GLU:O	2.37	0.41
1:DI:105:ARG:HH11	1:DI:140:ASN:HB3	1.86	0.41
1:EF:113:MET:HE1	1:EF:332:VAL:HG11	2.02	0.41
1:FD:285:PRO:HG2	1:GC:270:THR:H	1.85	0.41
1:FE:390:THR:O	1:FE:394:ILE:HG12	2.21	0.41
1:FH:379:ARG:HG3	1:FI:395:LEU:HD13	2.02	0.41
1:FI:70:ARG:NH2	1:FI:99:PHE:O	2.51	0.41
1:GB:164:PRO:HG3	1:GB:178:ASN:ND2	2.36	0.41
1:GE:52:LYS:HG2	1:GE:53:VAL:N	2.36	0.41
1:GF:201:LYS:HB3	1:GF:207:TRP:CE3	2.56	0.41
1:GH:274:ASN:OD1	1:GH:275:ILE:N	2.54	0.41
1:DF:372:VAL:O	1:DF:376:VAL:HG23	2.21	0.40
1:DJ:198:TYR:O	1:DJ:209:VAL:HA	2.21	0.40
1:DJ:379:ARG:HA	1:DJ:379:ARG:HD3	1.81	0.40
1:EA:174:ALA:HA	1:EA:177:TYR:CE1	2.57	0.40
1:EG:230:LYS:HD3	1:EG:239:SER:HB2	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FA:247:THR:OG1	1:FA:248:GLY:N	2.55	0.40
1:FC:70:ARG:HB2	1:FC:73:ASP:OD1	2.21	0.40
1:FH:72:LEU:HD23	1:FH:72:LEU:HA	1.87	0.40
1:FH:355:LEU:HD23	1:FH:355:LEU:HA	1.93	0.40
1:FI:287:ASP:OD1	1:FI:287:ASP:N	2.52	0.40
1:FK:305:ASN:O	1:FK:307:GLN:HG2	2.21	0.40
1:GD:173:ASP:OD2	1:GD:176:SER:N	2.54	0.40
1:GD:198:TYR:HE1	1:GD:212:HIS:HB3	1.86	0.40
1:GD:370:GLU:H	1:GD:370:GLU:CD	2.28	0.40
1:GI:139:PRO:HB2	1:GI:141:THR:HG23	2.02	0.40
1:DA:235:GLY:HA2	1:DA:267:GLN:HB3	2.03	0.40
1:DD:5:ALA:HB1	1:DD:388:ILE:HG12	2.02	0.40
1:DE:316:LEU:HD11	1:DE:355:LEU:HD11	2.03	0.40
1:DF:266:MET:HE1	1:DG:142:LEU:HD23	2.04	0.40
1:DH:251:ASN:C	1:DH:251:ASN:ND2	2.79	0.40
1:EB:73:ASP:N	1:EB:73:ASP:OD1	2.53	0.40
1:EE:241:GLY:HA2	1:EE:262:PHE:HB2	2.02	0.40
1:EI:367:LEU:HD23	1:EI:367:LEU:HA	1.90	0.40
1:FC:387:THR:HG23	1:FD:374:MET:HE1	2.03	0.40
1:FH:70:ARG:O	1:FH:358:GLY:HA2	2.21	0.40
1:GC:82:PHE:O	1:GC:93:TYR:HA	2.22	0.40
1:DE:177:TYR:CE2	1:DE:180:LYS:HB2	2.56	0.40
1:DF:199:PHE:HD1	1:DF:209:VAL:HG12	1.87	0.40
1:EC:5:ALA:HB1	1:EC:388:ILE:HG12	2.02	0.40
1:EH:232:ASN:HD21	1:EH:236:ILE:HG13	1.87	0.40
1:EJ:74:VAL:O	1:EJ:97:GLY:HA3	2.22	0.40
1:FE:159:SER:OG	1:FE:160:THR:N	2.55	0.40
1:FE:195:MET:HE2	1:FE:195:MET:HA	2.03	0.40
1:FG:261:SER:HB2	1:FG:263:LEU:HD23	2.03	0.40
1:GC:390:THR:O	1:GC:394:ILE:HG12	2.22	0.40
1:GD:94:SER:HB2	1:GD:332:VAL:HA	2.02	0.40
1:GH:378:GLN:HE21	1:GH:382:GLN:NE2	2.19	0.40
1:DA:155:ILE:HD11	1:DA:179:LYS:HG2	2.03	0.40
1:DC:169:PHE:HE1	1:DC:177:TYR:HB3	1.87	0.40
1:DD:94:SER:OG	1:DD:95:ARG:N	2.54	0.40
1:DF:169:PHE:HE2	1:DF:222:PRO:HG2	1.86	0.40
1:EC:45:SER:OG	1:EC:46:LYS:N	2.54	0.40
1:EC:118:TYR:HA	1:EC:119:PRO:HD3	1.96	0.40
1:EI:149:THR:OG1	1:EI:281:ASN:ND2	2.38	0.40
1:FA:158:ASN:C	1:FA:160:THR:H	2.28	0.40
1:FA:201:LYS:HB2	1:FA:207:TRP:CD2	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FB:70:ARG:HH22	1:FB:98:GLN:HG2	1.86	0.40
1:FH:68:THR:OG1	1:FH:73:ASP:OD2	2.35	0.40
1:GB:124:PRO:HA	1:GB:125:PRO:HD3	1.97	0.40
1:GC:72:LEU:HD11	1:GC:291:TYR:HE2	1.86	0.40
1:GC:149:THR:HG1	1:GC:281:ASN:HD21	1.63	0.40
1:GC:180:LYS:HE2	1:GC:180:LYS:HB3	1.85	0.40
1:GF:354:LYS:HB3	1:GF:354:LYS:HE2	1.93	0.40
1:GK:164:PRO:HG3	1:GK:200:VAL:HG13	2.02	0.40
1:GK:232:ASN:OD1	1:GK:236:ILE:N	2.54	0.40
1:DC:209:VAL:HG22	1:DC:227:THR:HB	2.03	0.40
1:DK:82:PHE:HB2	1:DK:94:SER:O	2.22	0.40
1:EF:345:GLY:HA3	1:EF:352:PHE:CE2	2.57	0.40
1:EJ:211:THR:HG21	1:EJ:245:ILE:HG21	2.03	0.40
1:EK:107:LEU:HD23	1:EK:107:LEU:HA	1.95	0.40
1:FH:170:SER:HB3	1:FH:173:ASP:HB3	2.03	0.40
1:GB:345:GLY:HA3	1:GB:352:PHE:CZ	2.57	0.40
1:GH:388:ILE:HD12	1:GH:388:ILE:H	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	DA	400/402 (100%)	388 (97%)	12 (3%)	0	100	100
1	DB	400/402 (100%)	388 (97%)	12 (3%)	0	100	100
1	DC	400/402 (100%)	390 (98%)	10 (2%)	0	100	100
1	DD	400/402 (100%)	389 (97%)	11 (3%)	0	100	100
1	DE	400/402 (100%)	389 (97%)	11 (3%)	0	100	100
1	DF	400/402 (100%)	379 (95%)	21 (5%)	0	100	100
1	DG	400/402 (100%)	386 (96%)	14 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	DH	400/402 (100%)	389 (97%)	11 (3%)	0	100	100
1	DI	400/402 (100%)	390 (98%)	10 (2%)	0	100	100
1	DJ	400/402 (100%)	389 (97%)	11 (3%)	0	100	100
1	DK	400/402 (100%)	388 (97%)	12 (3%)	0	100	100
1	EA	400/402 (100%)	391 (98%)	9 (2%)	0	100	100
1	EB	400/402 (100%)	390 (98%)	10 (2%)	0	100	100
1	EC	400/402 (100%)	389 (97%)	11 (3%)	0	100	100
1	ED	400/402 (100%)	388 (97%)	12 (3%)	0	100	100
1	EE	400/402 (100%)	388 (97%)	12 (3%)	0	100	100
1	EF	400/402 (100%)	381 (95%)	19 (5%)	0	100	100
1	EG	400/402 (100%)	389 (97%)	11 (3%)	0	100	100
1	EH	400/402 (100%)	388 (97%)	12 (3%)	0	100	100
1	EI	400/402 (100%)	389 (97%)	11 (3%)	0	100	100
1	EJ	400/402 (100%)	389 (97%)	11 (3%)	0	100	100
1	EK	400/402 (100%)	391 (98%)	9 (2%)	0	100	100
1	FA	400/402 (100%)	385 (96%)	15 (4%)	0	100	100
1	FB	400/402 (100%)	389 (97%)	11 (3%)	0	100	100
1	FC	400/402 (100%)	386 (96%)	13 (3%)	1 (0%)	36	66
1	FD	400/402 (100%)	390 (98%)	10 (2%)	0	100	100
1	FE	400/402 (100%)	386 (96%)	14 (4%)	0	100	100
1	FF	400/402 (100%)	379 (95%)	21 (5%)	0	100	100
1	FG	400/402 (100%)	383 (96%)	17 (4%)	0	100	100
1	FH	400/402 (100%)	384 (96%)	16 (4%)	0	100	100
1	FI	400/402 (100%)	387 (97%)	13 (3%)	0	100	100
1	FJ	400/402 (100%)	392 (98%)	8 (2%)	0	100	100
1	FK	400/402 (100%)	387 (97%)	13 (3%)	0	100	100
1	GA	400/402 (100%)	388 (97%)	12 (3%)	0	100	100
1	GB	400/402 (100%)	387 (97%)	13 (3%)	0	100	100
1	GC	400/402 (100%)	390 (98%)	10 (2%)	0	100	100
1	GD	400/402 (100%)	394 (98%)	5 (1%)	1 (0%)	36	66
1	GE	400/402 (100%)	385 (96%)	15 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	GF	400/402 (100%)	384 (96%)	16 (4%)	0	100	100
1	GG	400/402 (100%)	385 (96%)	15 (4%)	0	100	100
1	GH	400/402 (100%)	393 (98%)	7 (2%)	0	100	100
1	GI	400/402 (100%)	393 (98%)	7 (2%)	0	100	100
1	GJ	400/402 (100%)	389 (97%)	11 (3%)	0	100	100
1	GK	400/402 (100%)	390 (98%)	10 (2%)	0	100	100
All	All	17600/17688 (100%)	17064 (97%)	534 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	FC	124	PRO
1	GD	124	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	DA	322/322 (100%)	322 (100%)	0	100	100
1	DB	322/322 (100%)	322 (100%)	0	100	100
1	DC	322/322 (100%)	322 (100%)	0	100	100
1	DD	322/322 (100%)	322 (100%)	0	100	100
1	DE	322/322 (100%)	322 (100%)	0	100	100
1	DF	322/322 (100%)	321 (100%)	1 (0%)	86	86
1	DG	322/322 (100%)	322 (100%)	0	100	100
1	DH	322/322 (100%)	322 (100%)	0	100	100
1	DI	322/322 (100%)	322 (100%)	0	100	100
1	DJ	322/322 (100%)	322 (100%)	0	100	100
1	DK	322/322 (100%)	322 (100%)	0	100	100
1	EA	322/322 (100%)	322 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	EB	322/322 (100%)	322 (100%)	0	100	100
1	EC	322/322 (100%)	321 (100%)	1 (0%)	86	86
1	ED	322/322 (100%)	322 (100%)	0	100	100
1	EE	322/322 (100%)	322 (100%)	0	100	100
1	EF	322/322 (100%)	322 (100%)	0	100	100
1	EG	322/322 (100%)	322 (100%)	0	100	100
1	EH	322/322 (100%)	322 (100%)	0	100	100
1	EI	322/322 (100%)	322 (100%)	0	100	100
1	EJ	322/322 (100%)	321 (100%)	1 (0%)	86	86
1	EK	322/322 (100%)	322 (100%)	0	100	100
1	FA	322/322 (100%)	322 (100%)	0	100	100
1	FB	322/322 (100%)	322 (100%)	0	100	100
1	FC	322/322 (100%)	322 (100%)	0	100	100
1	FD	322/322 (100%)	322 (100%)	0	100	100
1	FE	322/322 (100%)	322 (100%)	0	100	100
1	FF	322/322 (100%)	322 (100%)	0	100	100
1	FG	322/322 (100%)	321 (100%)	1 (0%)	86	86
1	FH	322/322 (100%)	322 (100%)	0	100	100
1	FI	322/322 (100%)	322 (100%)	0	100	100
1	FJ	322/322 (100%)	322 (100%)	0	100	100
1	FK	322/322 (100%)	322 (100%)	0	100	100
1	GA	322/322 (100%)	322 (100%)	0	100	100
1	GB	322/322 (100%)	321 (100%)	1 (0%)	86	86
1	GC	322/322 (100%)	322 (100%)	0	100	100
1	GD	322/322 (100%)	322 (100%)	0	100	100
1	GE	322/322 (100%)	322 (100%)	0	100	100
1	GF	322/322 (100%)	322 (100%)	0	100	100
1	GG	322/322 (100%)	322 (100%)	0	100	100
1	GH	322/322 (100%)	322 (100%)	0	100	100
1	GI	322/322 (100%)	322 (100%)	0	100	100
1	GJ	322/322 (100%)	322 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	GK	322/322 (100%)	322 (100%)	0	100	100
All	All	14168/14168 (100%)	14163 (100%)	5 (0%)	100	100

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	DF	264	ASN
1	EC	78	GLN
1	EJ	140	ASN
1	FG	251	ASN
1	GB	391	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (177) such sidechains are listed below:

Mol	Chain	Res	Type
1	DA	274	ASN
1	DA	318	ASN
1	DA	400	ASN
1	DB	328	GLN
1	DC	251	ASN
1	DD	114	GLN
1	DD	251	ASN
1	DE	132	ASN
1	DE	205	ASN
1	DF	244	ASN
1	DF	267	GLN
1	DF	268	GLN
1	DF	313	GLN
1	DG	96	ASN
1	DG	196	ASN
1	DG	294	ASN
1	DG	302	ASN
1	DG	328	GLN
1	DH	114	GLN
1	DH	178	ASN
1	DH	232	ASN
1	DH	321	ASN
1	DH	331	ASN
1	DH	391	GLN
1	DI	154	GLN
1	DI	294	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	DJ	25	ASN
1	DJ	58	GLN
1	DJ	67	ASN
1	DJ	212	HIS
1	DJ	267	GLN
1	DJ	295	ASN
1	DJ	331	ASN
1	DJ	386	GLN
1	DK	58	GLN
1	DK	212	HIS
1	DK	318	ASN
1	DK	384	ASN
1	EA	106	ASN
1	EA	268	GLN
1	EA	305	ASN
1	EA	328	GLN
1	EA	331	ASN
1	EB	212	HIS
1	EB	295	ASN
1	EB	328	GLN
1	EB	400	ASN
1	EC	96	ASN
1	EC	251	ASN
1	EC	364	ASN
1	ED	67	ASN
1	ED	364	ASN
1	ED	378	GLN
1	EE	67	ASN
1	EE	128	GLN
1	EE	212	HIS
1	EE	357	ASN
1	EF	78	GLN
1	EF	96	ASN
1	EF	98	GLN
1	EF	212	HIS
1	EF	274	ASN
1	EF	292	GLN
1	EF	294	ASN
1	EF	307	GLN
1	EF	318	ASN
1	EG	25	ASN
1	EG	96	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	EG	111	GLN
1	EH	302	ASN
1	EH	309	GLN
1	EH	331	ASN
1	EI	309	GLN
1	EI	331	ASN
1	EI	386	GLN
1	EJ	21	ASN
1	EJ	264	ASN
1	EK	114	GLN
1	EK	189	GLN
1	EK	318	ASN
1	EK	328	GLN
1	EK	386	GLN
1	FA	67	ASN
1	FA	78	GLN
1	FA	251	ASN
1	FB	88	ASN
1	FB	104	ASN
1	FB	302	ASN
1	FB	328	GLN
1	FB	357	ASN
1	FB	386	GLN
1	FB	400	ASN
1	FC	88	ASN
1	FC	106	ASN
1	FC	178	ASN
1	FC	234	ASN
1	FC	357	ASN
1	FC	386	GLN
1	FD	191	ASN
1	FD	196	ASN
1	FD	280	GLN
1	FD	378	GLN
1	FD	384	ASN
1	FD	386	GLN
1	FD	400	ASN
1	FE	58	GLN
1	FE	96	ASN
1	FE	234	ASN
1	FE	273	ASN
1	FE	321	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	FE	328	GLN
1	FF	96	ASN
1	FF	302	ASN
1	FF	318	ASN
1	FF	321	ASN
1	FF	351	ASN
1	FG	78	GLN
1	FG	114	GLN
1	FG	234	ASN
1	FG	302	ASN
1	FH	67	ASN
1	FH	96	ASN
1	FH	178	ASN
1	FH	251	ASN
1	FH	302	ASN
1	FI	212	HIS
1	FI	357	ASN
1	FI	400	ASN
1	FJ	178	ASN
1	FJ	191	ASN
1	FJ	351	ASN
1	FJ	386	GLN
1	FJ	396	ASN
1	FK	96	ASN
1	FK	128	GLN
1	FK	280	GLN
1	FK	400	ASN
1	GA	104	ASN
1	GA	191	ASN
1	GB	114	GLN
1	GB	191	ASN
1	GB	328	GLN
1	GB	378	GLN
1	GB	391	GLN
1	GC	212	HIS
1	GD	98	GLN
1	GD	191	ASN
1	GD	373	ASN
1	GD	391	GLN
1	GD	393	GLN
1	GE	21	ASN
1	GE	106	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	GE	129	GLN
1	GE	309	GLN
1	GE	328	GLN
1	GF	25	ASN
1	GF	193	HIS
1	GF	196	ASN
1	GF	234	ASN
1	GF	244	ASN
1	GF	318	ASN
1	GG	25	ASN
1	GG	98	GLN
1	GH	132	ASN
1	GH	382	GLN
1	GH	396	ASN
1	GI	128	GLN
1	GI	205	ASN
1	GI	212	HIS
1	GJ	67	ASN
1	GJ	264	ASN
1	GJ	267	GLN
1	GJ	382	GLN
1	GK	114	GLN
1	GK	178	ASN
1	GK	378	GLN
1	GK	382	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

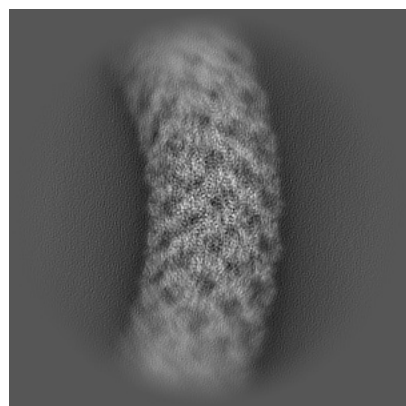
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63690. These allow visual inspection of the internal detail of the map and identification of artifacts.

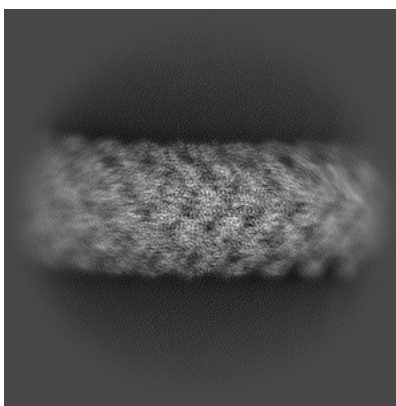
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

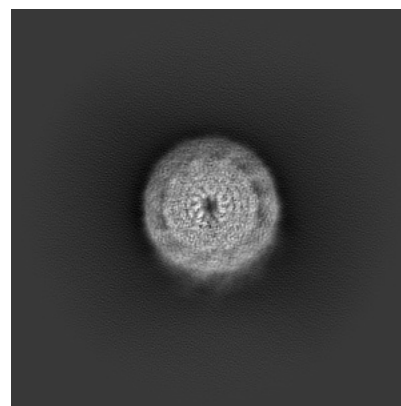
6.1.1 Primary map



X

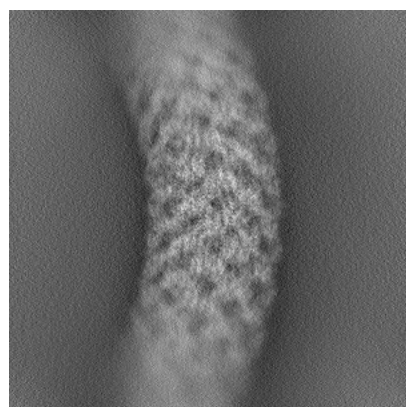


Y

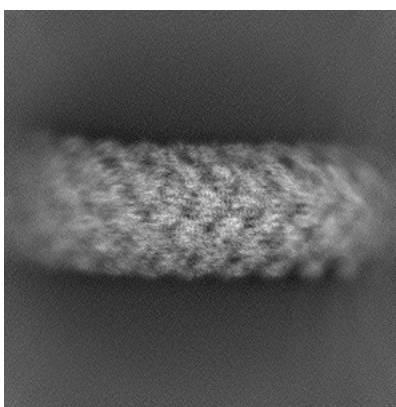


Z

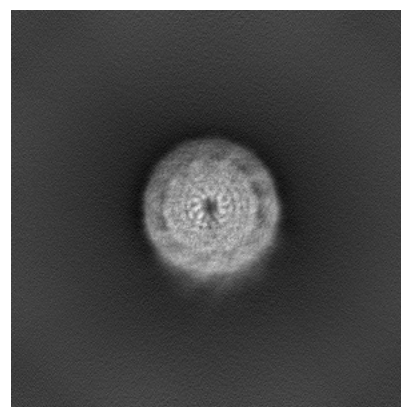
6.1.2 Raw map



X



Y

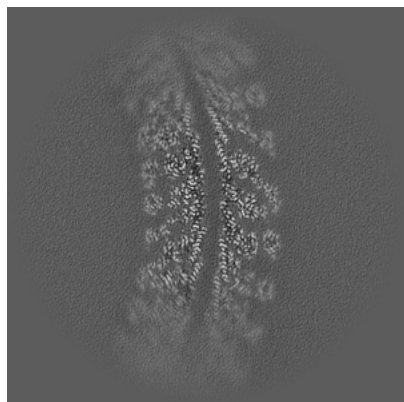


Z

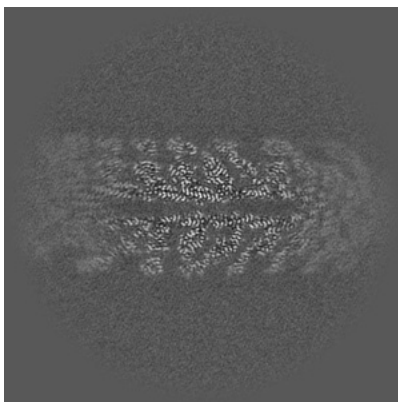
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

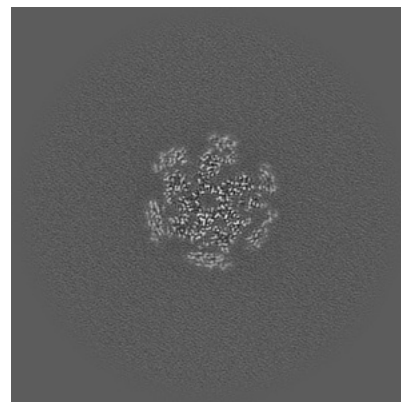
6.2.1 Primary map



X Index: 300

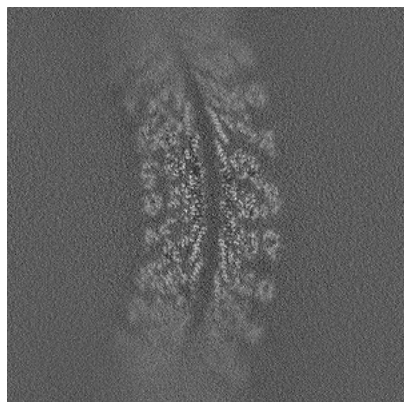


Y Index: 300

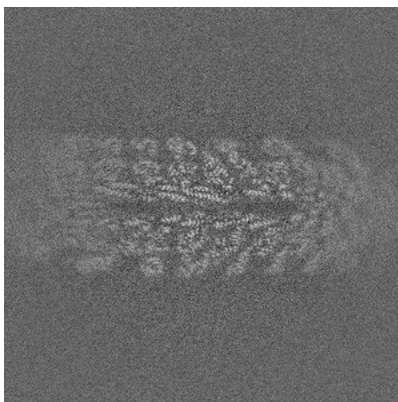


Z Index: 300

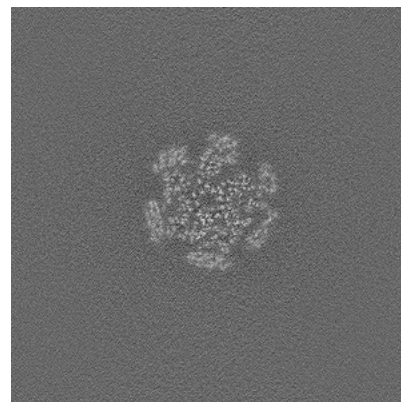
6.2.2 Raw map



X Index: 300



Y Index: 300

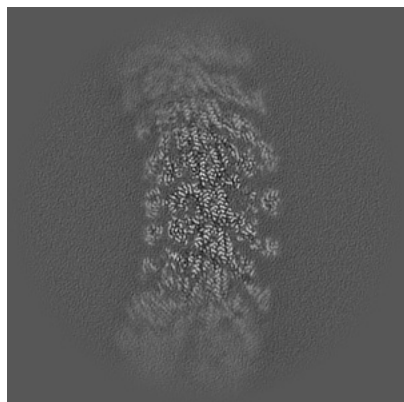


Z Index: 300

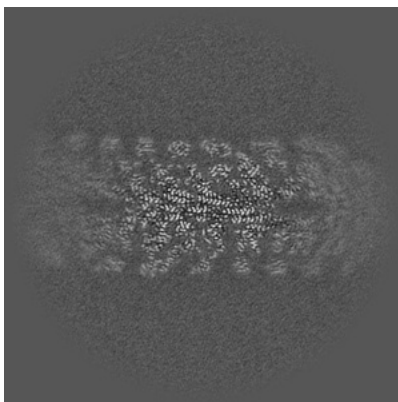
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

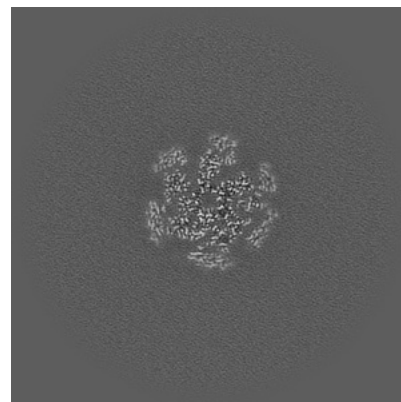
6.3.1 Primary map



X Index: 314

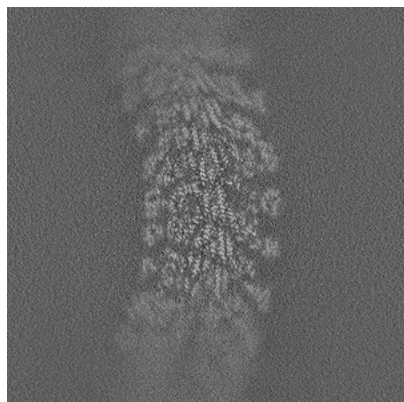


Y Index: 287

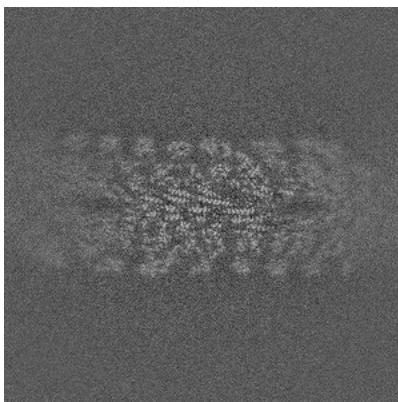


Z Index: 301

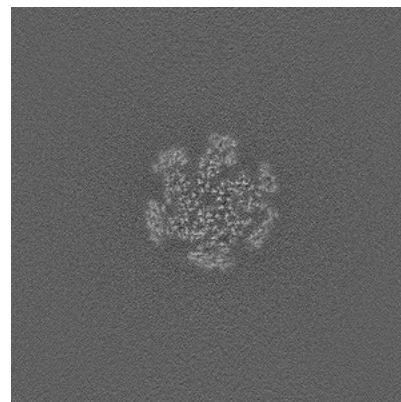
6.3.2 Raw map



X Index: 314



Y Index: 287

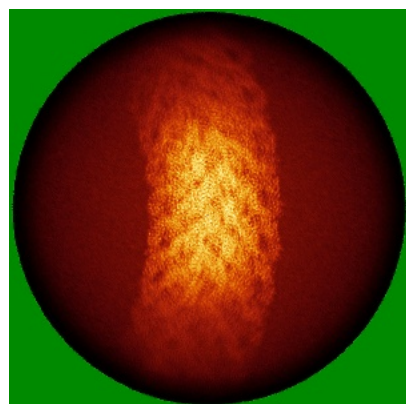


Z Index: 301

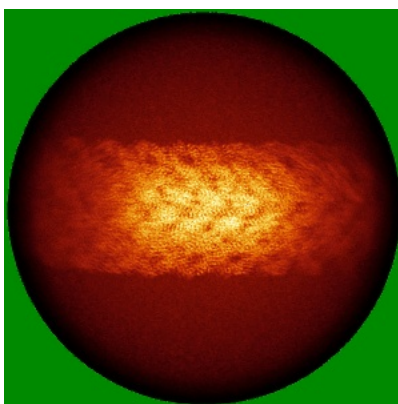
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

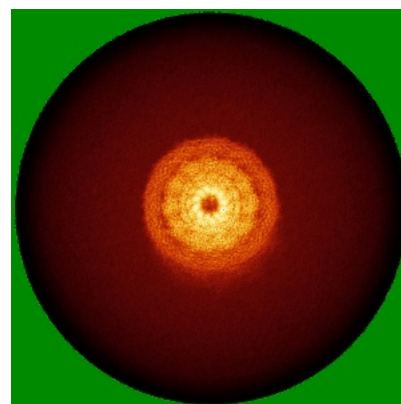
6.4.1 Primary map



X

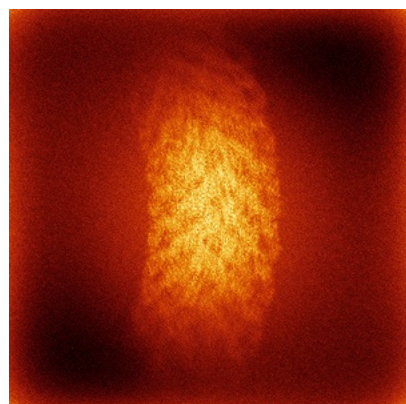


Y

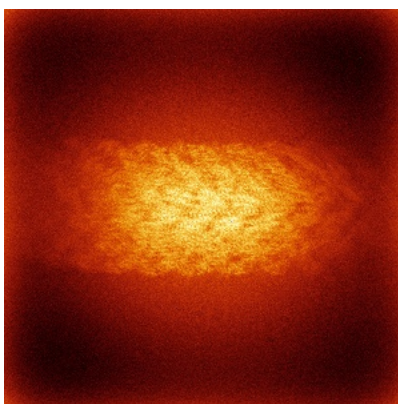


Z

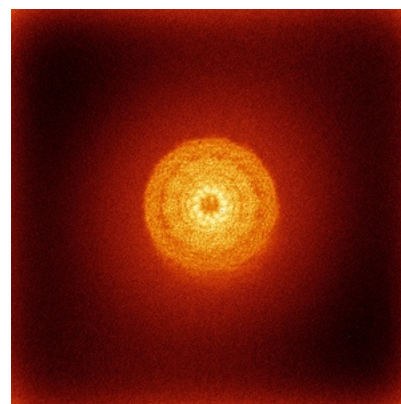
6.4.2 Raw map



X



Y

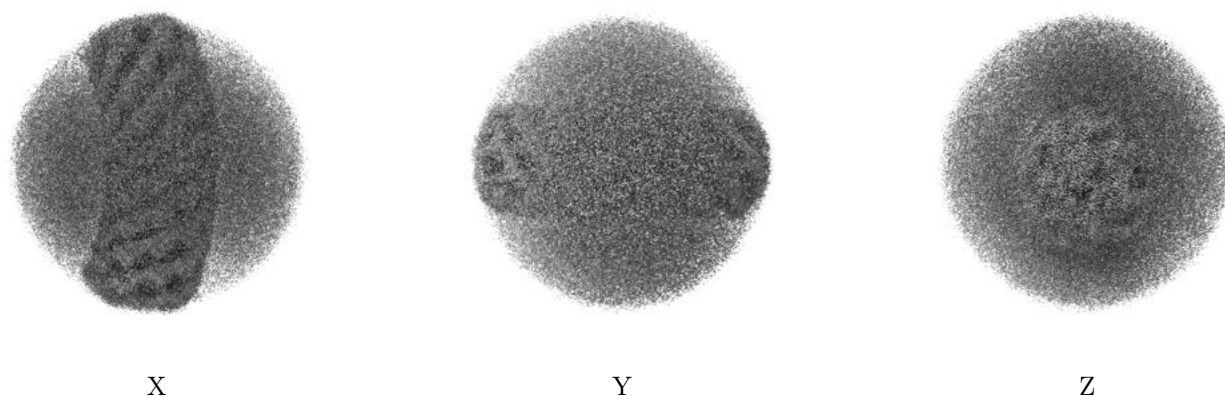


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.075. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

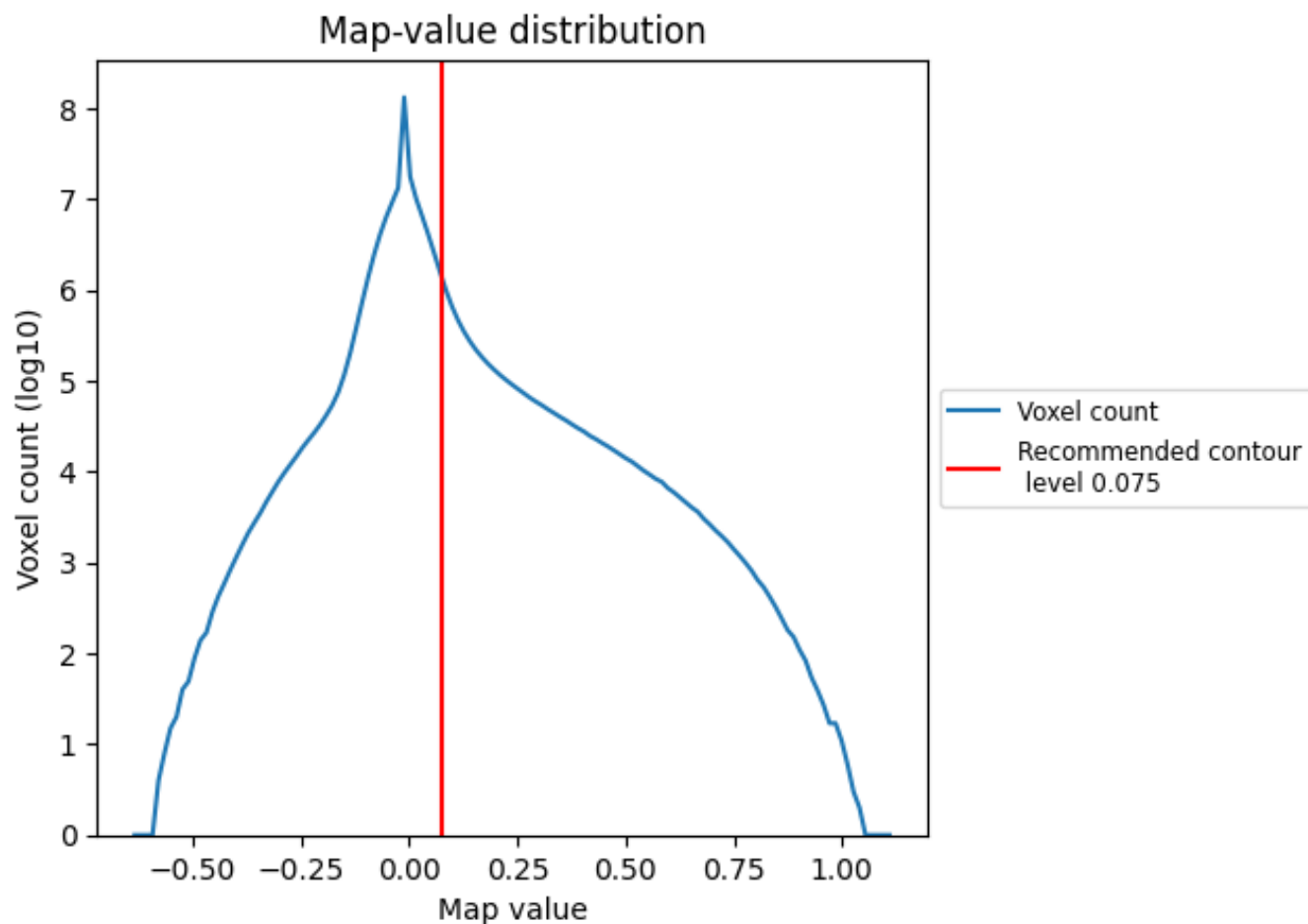
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

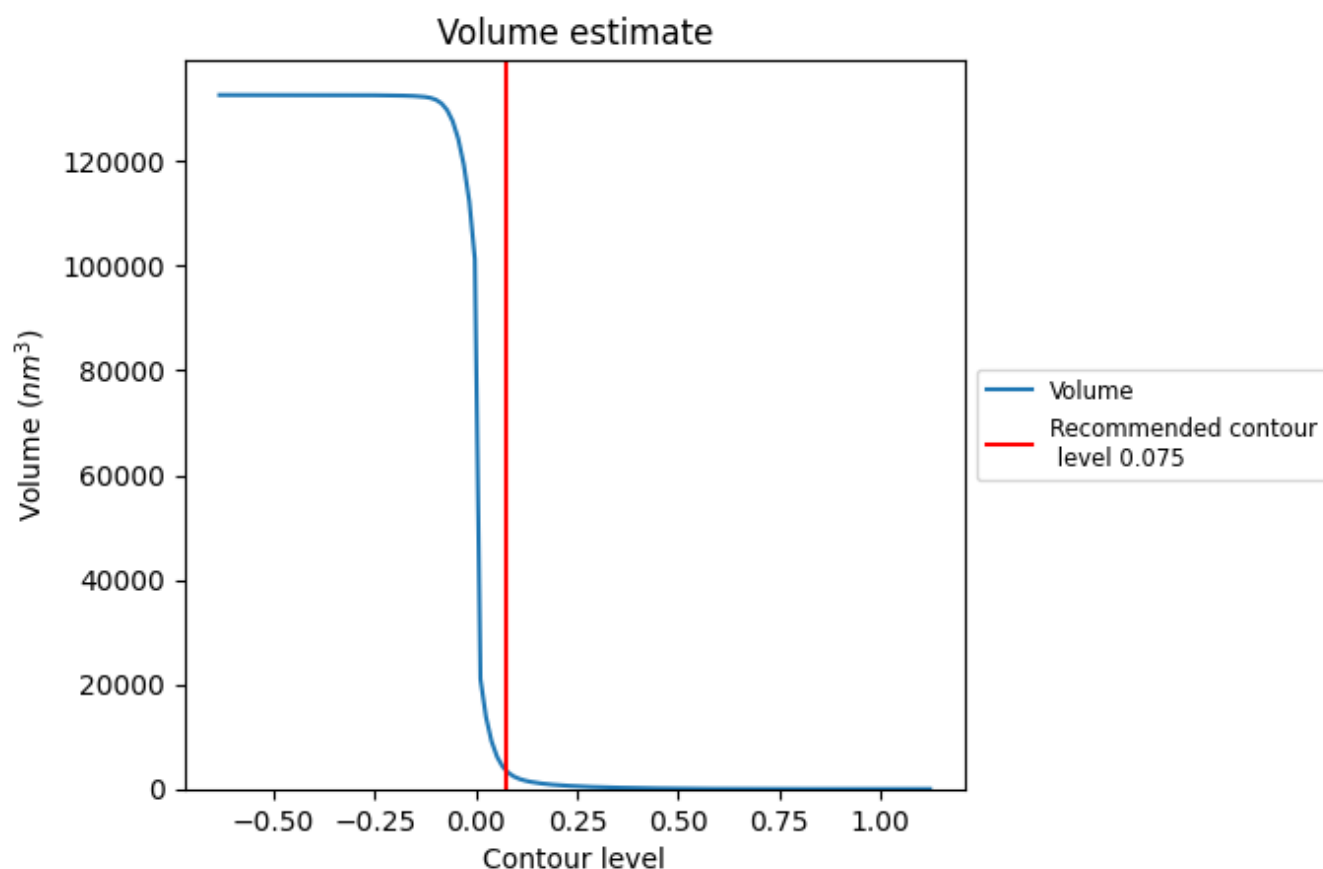
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

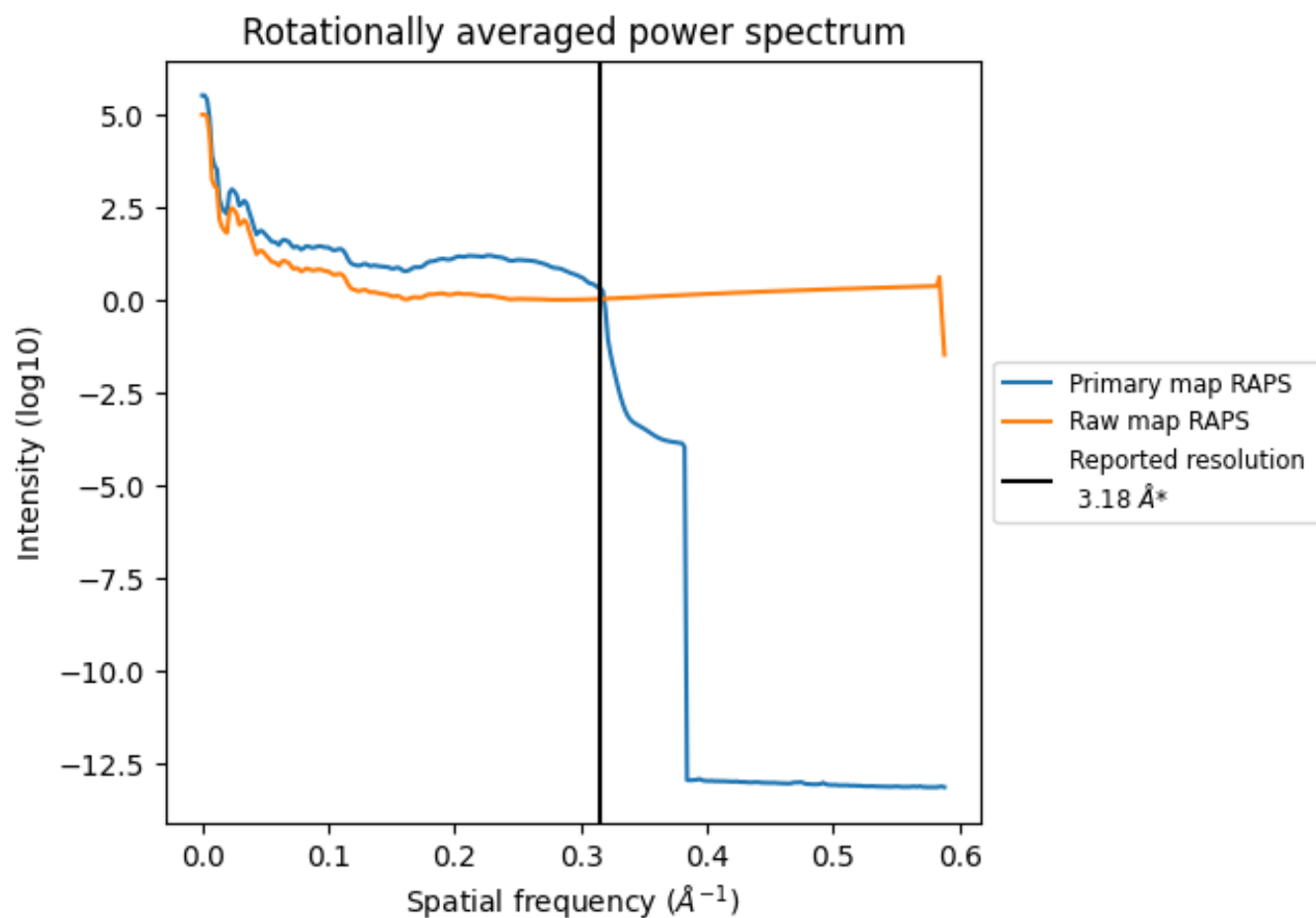
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3496 nm^3 ; this corresponds to an approximate mass of 3158 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

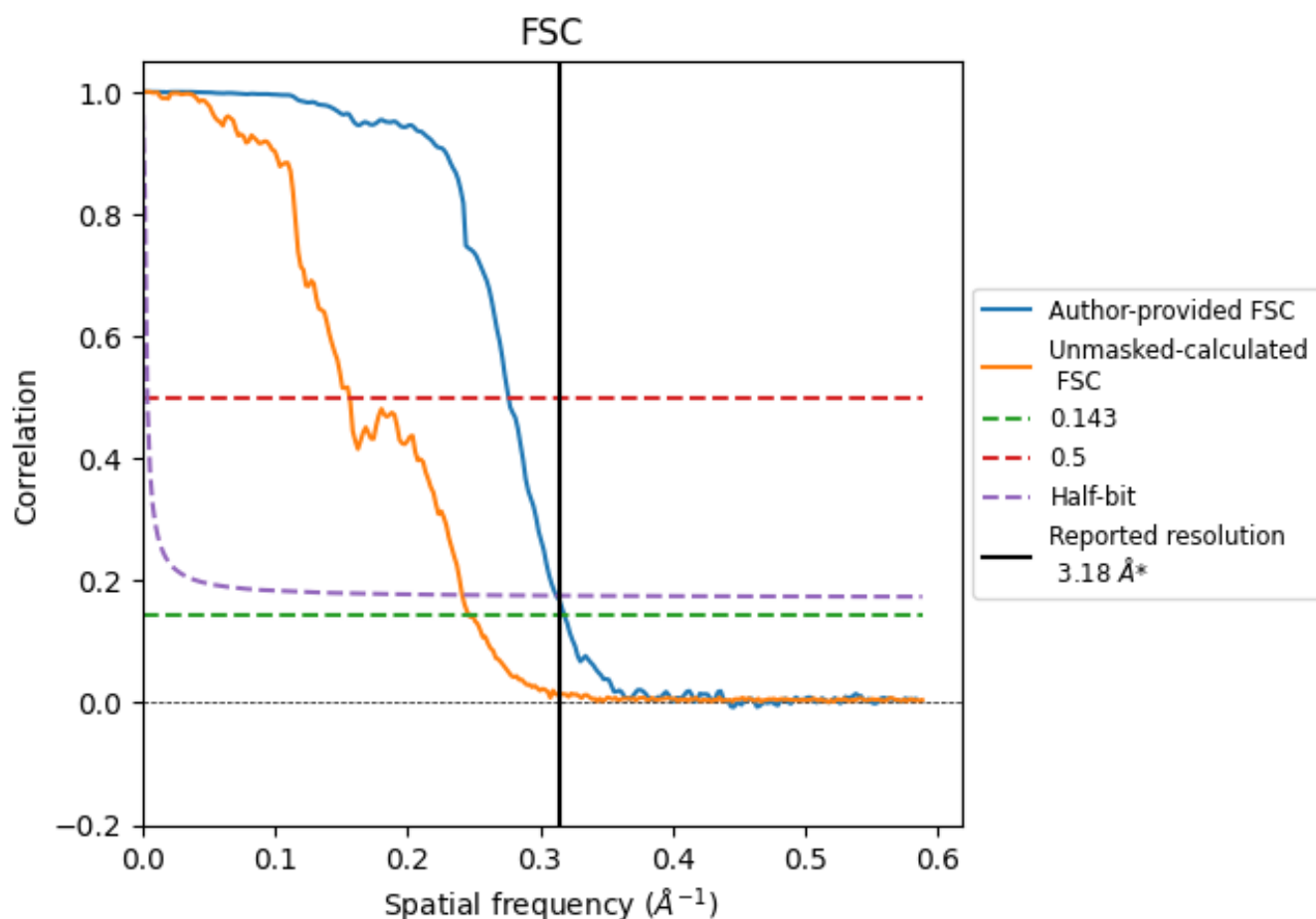


*Reported resolution corresponds to spatial frequency of 0.314 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.314 \AA^{-1}

8.2 Resolution estimates [i](#)

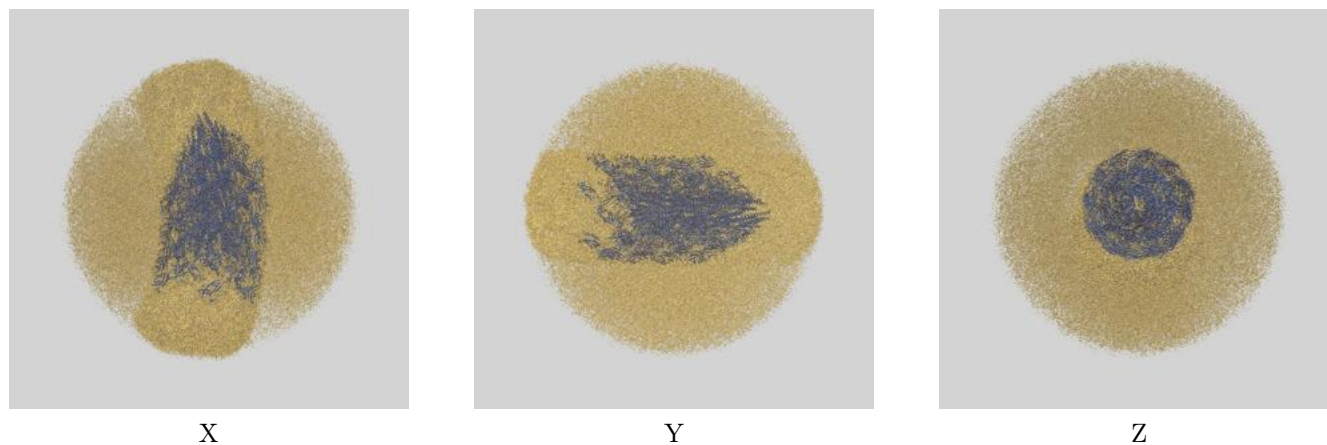
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.18	-	-
Author-provided FSC curve	3.14	3.62	3.20
Unmasked-calculated*	4.06	6.40	4.14

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.06 differs from the reported value 3.18 by more than 10 %

9 Map-model fit [i](#)

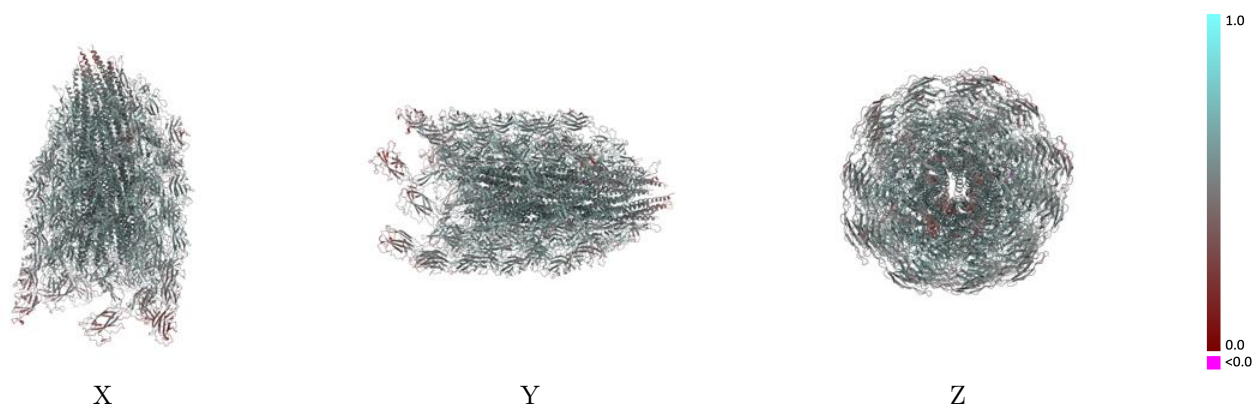
This section contains information regarding the fit between EMDB map EMD-63690 and PDB model 9M7Q. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



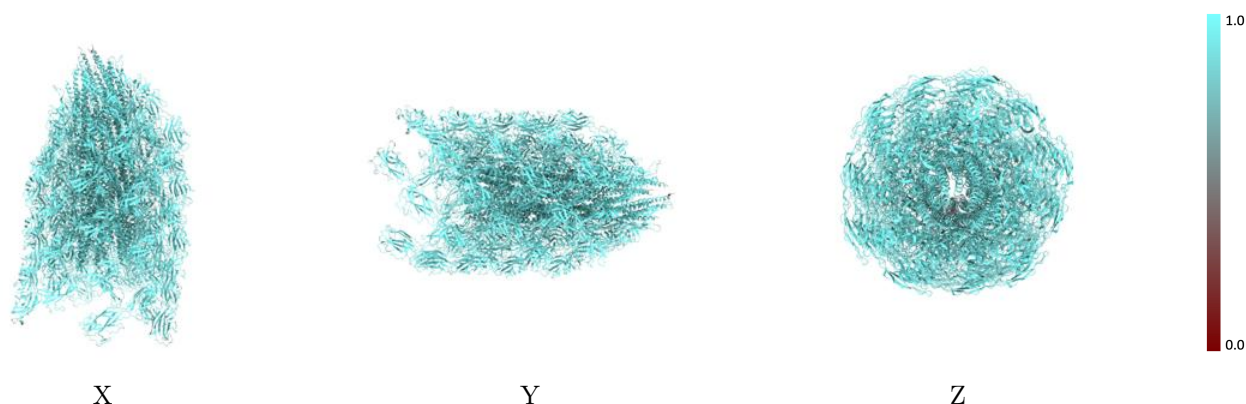
The images above show the 3D surface view of the map at the recommended contour level 0.075 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



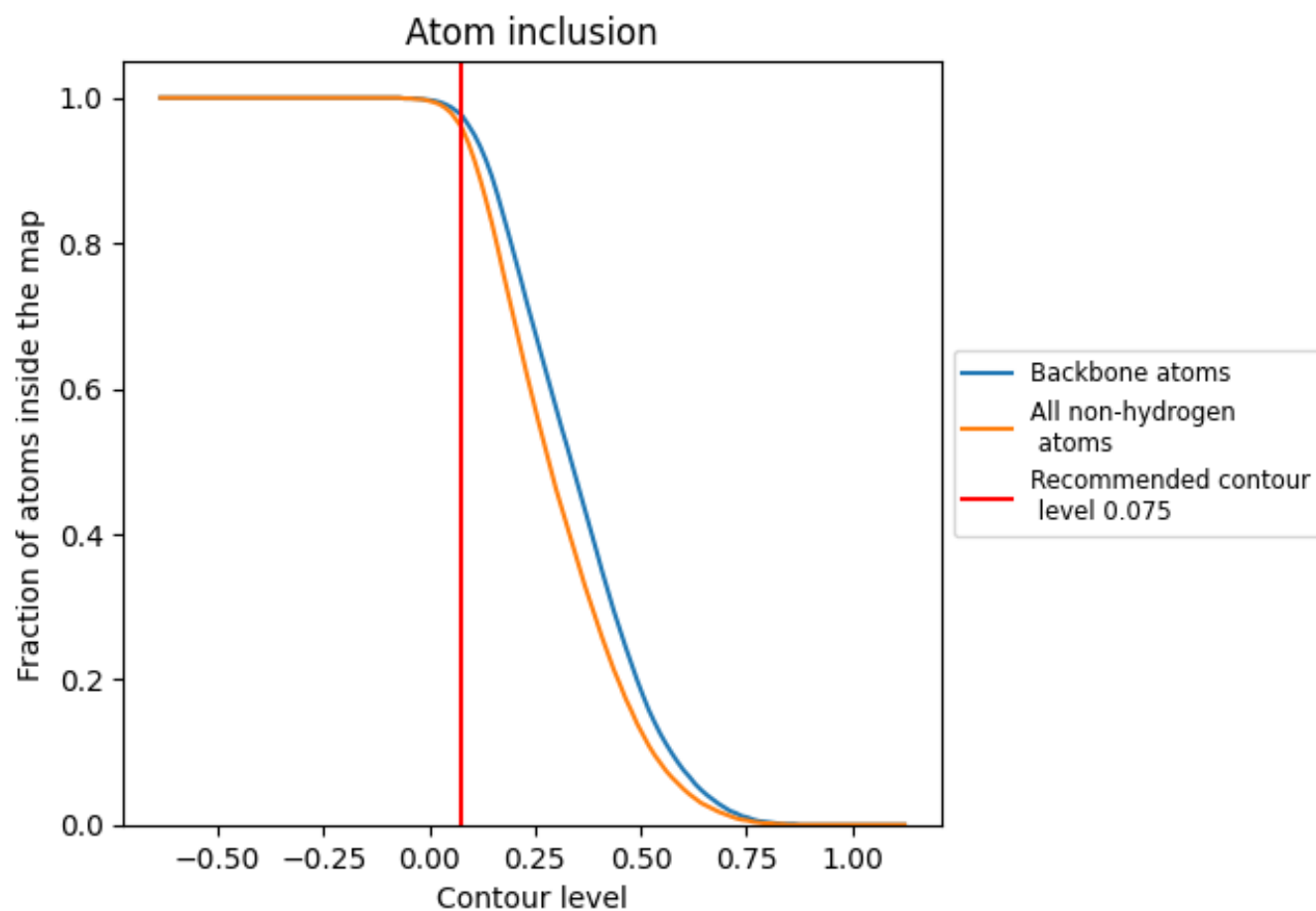
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.075).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary





















The table lists the average atom inclusion at the recommended contour level (0.075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9610	 0.5220
DA	 0.9260	 0.4820
DB	 0.9560	 0.5120
DC	 0.9510	 0.5000
DD	 0.9600	 0.5210
DE	 0.9500	 0.4990
DF	 0.9620	 0.5180
DG	 0.9320	 0.4830
DH	 0.9500	 0.5080
DI	 0.9170	 0.4540
DJ	 0.9510	 0.5080
DK	 0.9220	 0.4700
EA	 0.9660	 0.5280
EB	 0.9710	 0.5420
EC	 0.9750	 0.5440
ED	 0.9720	 0.5480
EE	 0.9740	 0.5430
EF	 0.9740	 0.5490
EG	 0.9730	 0.5390
EH	 0.9770	 0.5420
EI	 0.9720	 0.5320
EJ	 0.9750	 0.5440
EK	 0.9650	 0.5350
FA	 0.9710	 0.5480
FB	 0.9740	 0.5560
FC	 0.9760	 0.5570
FD	 0.9720	 0.5470
FE	 0.9750	 0.5500
FF	 0.9720	 0.5390
FG	 0.9740	 0.5420
FH	 0.9700	 0.5330
FI	 0.9750	 0.5460
FJ	 0.9730	 0.5450
FK	 0.9740	 0.5530
GA	 0.9750	 0.5430



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
GB	 0.9520	 0.5090
GC	 0.9640	 0.5280
GD	 0.9290	 0.4780
GE	 0.9630	 0.5210
GF	 0.9310	 0.4550
GG	 0.9650	 0.5100
GH	 0.9430	 0.4550
GI	 0.9690	 0.5140
GJ	 0.9510	 0.4940
GK	 0.9650	 0.5350